# Symmetries of Four Harmonically-Trapped Particles in One Dimension 

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#### Abstract

We present a method for solving interacting, four-body systems in a one-dimensional harmonic trap. By expressing the particle coordinates in Jacobi cartesian coordinates, we discover the underlying $O_{h}$ symmetry, i.e. tetrahedral $\left(T_{d}\right)$ symmetry with parity inversion. This symmetry provides an alternate method for describing particle configurations and clustering, and it simplifies numerical calculations of the energy eigenstates of the system for tunable interactions.


## I. INTRODUCTION

Recent advances in experimental measurements of ultracold, trapped, and interacting few-body systems have generated a need for precision calculations in few-body physics [110]. Experimental progress motivates theoretical work, and precise theoretical models allow for the advancement of experimental measurements [11].

In our theoretical model, we develop an efficient method to solve for the spectrum of the Hamiltonian in a truncated Hilbert space. The three-particle method in [1] simplifies the calculation of the Hamiltonian's energy eigenstates by exploiting the underlying $C_{6 v}$ symmetry (i.e., hexagonal symmetry with a vertical reflection plane). Building on this three-particle method, we present a method for solving four harmonically-trapped particles in one dimension by using an optimal computational basis that exploits the Hamiltonian's underlying $O_{h}$ symmetry (i.e. tetrahedral $\left(T_{d}\right)$ symmetry with parity inversion) and reduces the number of degrees of freedom from four to three. Additionally, our model conveniently describes particle clustering and interactions.

This method has a long history in nuclear, atomic, and molecular physics. Refs. [2] and [3] exploit similar properties using different methods, and ref. [4] solves a similar problem using an alternate, but related approach. Recent theoretical and experimental research has also provided evidence for an analogous Efimov effect in the unitary limit of the $N>3$-body problem, opening a vast new domain of research in many-body systems [12].

## II. MODEL OVERVIEW

In Sections III, IV, and V we begin by deriving the Hamiltonian for the harmonic trap potentials and interaction potentials in two-, three-, and four-particle systems. The trap potential contains energy potentials arising only from the trap itself, whereas the interaction potential contains only the contact potentials between two-particle interactions.

In each of the following derivations we begin in the particle coordinate system in configuration space and perform a change of basis transformation into a Jacobi coordinate system, still in configuration space. Graphically, this change of basis transformation is simply a rotation of the coordinate axes in configuration space.

Starting with the two-particle system we derive the Hamiltonians in both bases and
present a variable change that creates analogous, unitless Hamiltonians. In the three- and four-particle systems we continue the derivation and present the Jacobi transformations for those systems.

## III. TWO-PARTICLE INTERACTION IN A ONE-DIMENSIONAL TRAP

## A. Hamiltonian in the Two-Dimensional Particle Basis

For two identical particles in a one-dimensional harmonic trap, the non-interacting Hamiltonian $H_{0}$ is given by

$$
\begin{equation*}
H_{0}=\frac{1}{2 m}{\tilde{p_{1}}}^{2}+\frac{1}{2 m}{\tilde{p_{2}}}^{2}+\frac{1}{2} k{\tilde{q_{1}}}^{2}+\frac{1}{2} k{\tilde{q_{2}}}^{2} \tag{1}
\end{equation*}
$$

and the two-particle contact interaction potential $V$ is given by

$$
\begin{equation*}
V=g\left(\delta\left(\tilde{q}_{1}-\tilde{q}_{2}\right)\right) \tag{2}
\end{equation*}
$$

where $\tilde{p}_{i}$ and $\tilde{q}_{i}$ are the momentum and position of particle $i$, and $g$ is a constant determined by the interaction strength.

In order to define unitless analogs to $H_{0}$ and $V$ we define a new quantity $\sigma$, a fundamental length scale, as

$$
\sigma=\sqrt{\frac{\hbar}{m \omega}}
$$

where $\omega=\sqrt{k / m}$. Using $\sigma$ we can define unitless analogs to $\tilde{q}_{i}$ and $\tilde{p}_{i}$ :

$$
\begin{equation*}
q_{i}=\frac{\tilde{q}_{i}}{\sigma}, \quad p_{i}=\frac{\tilde{p}_{i}}{\hbar / \sigma} \tag{3}
\end{equation*}
$$

Substituting these values into Equations 1 and 2 yields

$$
\begin{gathered}
H_{0}=\frac{1}{2} \hbar \omega\left(p_{1}^{2}+p_{2}^{2}+q_{1}^{2}+q_{2}^{2}\right), \text { and } \\
V=g\left(\delta\left(\sigma q_{1}-\sigma q_{2}\right)\right)=\frac{g}{\sigma}\left(\delta\left(q_{1}-q_{2}\right)\right) .
\end{gathered}
$$

We can finally define a unitless total Hamiltonian as

$$
\begin{aligned}
H_{g} & =\frac{H_{0}+V}{\hbar \omega} \\
& =\frac{1}{2}\left(p_{1}^{2}+p_{2}^{2}+q_{1}^{2}+q_{2}^{2}\right)+\gamma\left(\delta\left(q_{1}-q_{2}\right)\right)
\end{aligned}
$$

where $\gamma=g /(\hbar \omega \sigma)$.

## B. Hamiltonian in the Two-Dimensional Jacobi Basis

The particle space coordinates can be transformed into Jacobi space coordinates by the rotation matrix

$$
J_{2}=\left(\begin{array}{cc}
\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\
\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}
\end{array}\right)
$$

which rotates the coordinate axes by $-\frac{\pi}{4}$ radians as shown in Figure 1. When $J_{2}$ acts on the $\left(q_{1}, q_{2}\right)^{\top}$ position vector, we define a Jacobi coordinate basis in configuration space.

$$
J_{2}\binom{q_{1}}{q_{2}}=\binom{\frac{1}{\sqrt{2}} q_{1}-\frac{1}{\sqrt{2}} q_{2}}{\frac{1}{\sqrt{2}} q_{1}+\frac{1}{\sqrt{2}} q_{2}}=\binom{r_{1}}{r_{2}}
$$

That is, $J_{2} \boldsymbol{q}=\boldsymbol{r}$. Similarly, for the momentum coordinate in particle space we can define a coordinate in Jacobi space using the same transformation, i.e. $J_{2} \boldsymbol{p}=\boldsymbol{k}$. Thus, in Jacobi space, the total, unitless Hamiltonian is

$$
\begin{aligned}
H_{g} & =\frac{1}{2}\left(k_{1}^{2}+k_{2}^{2}+r_{1}^{2}+r_{2}^{2}\right)+\gamma\left(\delta\left(\sqrt{2} r_{1}\right)\right) \\
& =\frac{1}{2}\left(k_{1}^{2}+k_{2}^{2}+r_{1}^{2}+r_{2}^{2}\right)+\frac{\gamma}{\sqrt{2}}\left(\delta\left(r_{1}\right)\right)
\end{aligned}
$$



FIG. 1: This figure demonstrates that the transformation to Jacobi coordinates can be represented as a rotation in configuration space. The $r_{2}$ direction bisects the angle bounded by the all-positive $q_{1}-q_{2}$ quadrant.

## IV. THREE-PARTICLE INTERACTION IN A ONE-DIMENSIONAL TRAP

## A. Hamiltonian in the Three-Dimensional Particle Basis

A similar derivation exists for the three-particle case. In Jacobi space, the non-interacting Hamiltonian $H_{0}$ is given by

$$
H_{0}=\frac{1}{2 m}\left({\tilde{p_{1}}}^{2}+{\tilde{p_{2}}}^{2}+{\tilde{p_{3}}}^{2}\right)+\frac{1}{2} k\left({\tilde{q_{1}}}^{2}+{\tilde{q_{2}}}^{2}+{\tilde{q_{3}}}^{2}\right),
$$

and the three-particle contact interaction $V$ is given by

$$
V=g\left(\delta\left(\tilde{q_{1}}-\tilde{q_{2}}\right)+\delta\left(\tilde{q_{2}}-\tilde{q_{3}}\right)+\delta\left(\tilde{q_{3}}-\tilde{q_{1}}\right)\right) .
$$

Using the definitions assigned in Equation 3, we can, once again, find unitless analogs to $H_{0}$ and $V$, now in three dimensions. Here,

$$
\begin{aligned}
H_{0} & =\frac{1}{2} \hbar \omega\left(p_{1}^{2}+p_{2}^{2}+p_{3}^{2}+q_{1}^{2}+q_{2}^{2}+q_{3}^{2}\right) \\
& =\frac{1}{2} \hbar \omega\left(\boldsymbol{p}^{2}+\boldsymbol{q}^{2}\right), \text { and } \\
V= & \frac{g}{\sigma}\left(\delta\left(q_{1}-q_{2}\right)+\delta\left(q_{2}-q_{3}\right)+\delta\left(q_{3}-q_{1}\right)\right),
\end{aligned}
$$

where we've defined $\boldsymbol{p}=\left(p_{1}, p_{2}, p_{3}\right)^{\top}$ and $\boldsymbol{q}=\left(q_{1}, q_{2}, q_{3}\right)^{\top}$ for the three-particle case.


FIG. 2: This figure demonstrates that the transformation to Jacobi coordinates can be represented as a rotation in configuration space. The $r_{3}$ direction points into the middle of the solid angle bounded by the all-positive $q_{1}-q_{2}-q_{3}$ octant.

We can now define the unitless total Hamiltonian in three-dimensions as

$$
\begin{aligned}
H_{g}= & \frac{H_{0}+V}{\hbar \omega} \\
= & \frac{1}{2}\left(\boldsymbol{p}^{2}+\boldsymbol{q}^{2}\right) \\
& +\gamma\left(\delta\left(q_{1}-q_{2}\right)+\delta\left(q_{2}-q_{3}\right)+\delta\left(q_{3}-q_{1}\right)\right) .
\end{aligned}
$$

## B. Hamiltonian in Three-Dimensional Jacobi Space

The particle space coordinates can be transformed into Jacobi space coordinates by the rotation matrix

$$
J_{3}=\left(\begin{array}{ccc}
\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\
\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & -\sqrt{\frac{2}{3}} \\
\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}}
\end{array}\right)
$$

which rotates the coordinate axes by $-\frac{\pi}{4}$ radians in the azimuthal direction and then by $\frac{\pi}{4}$ radians in the polar direction as shown in Figure 2.

Similar to the transformation in 2-dimensions, $J_{3} \boldsymbol{q}=\boldsymbol{r}$ and $J_{3} \boldsymbol{p}=\boldsymbol{k}$. Thus, in three-
dimensional Jacobi space, the total, unitless Hamiltonian is

$$
\begin{aligned}
H_{g}= & \frac{1}{2}\left(\boldsymbol{k}^{2}+\boldsymbol{r}^{2}\right) \\
& +\gamma\left[\delta\left(\sqrt{2} r_{1}\right)+\delta\left(-\frac{1}{\sqrt{2}} r_{1}+\sqrt{\frac{3}{2}} r_{2}\right)\right. \\
& \left.+\delta\left(-\frac{1}{\sqrt{2}} r_{1}-\sqrt{\frac{3}{2}} r_{2}\right)\right],
\end{aligned}
$$

where $\boldsymbol{k}=\left(k_{1}, k_{2}, k_{3}\right)^{\top}$ and $\boldsymbol{r}=\left(r_{1}, r_{2}, r_{3}\right)^{\top}$ in three dimensions.

## V. FOUR-PARTICLE INTERACTION IN A ONE-DIMENSIONAL TRAP

## A. Hamiltonian in Four-Dimensional Particle Space

Finally, a similar derivation exists for the four-particle case. In particle space, the noninteracting Hamiltonian $H_{0}$ is given by

$$
\begin{align*}
H_{0}= & \frac{1}{2 m}\left({\tilde{p_{1}}}^{2}+{\tilde{p_{2}}}^{2}+{\tilde{p_{3}}}^{2}+{\tilde{p_{4}}}^{2}\right) \\
& +\frac{1}{2} k\left({\tilde{q_{1}}}^{2}+{\tilde{q_{2}}}^{2}+{\tilde{q_{3}}}^{2}+{\tilde{q_{4}}}^{2}\right) \\
= & \frac{1}{2 m} \tilde{\boldsymbol{P}}^{2}+\frac{1}{2} k \tilde{\boldsymbol{Q}}^{2}, \tag{4}
\end{align*}
$$

and the four-particle contact interaction $V$ is given by

$$
\begin{equation*}
V=g\left(\sum_{i=1}^{4} \sum_{j>i}^{4} \delta\left(\tilde{q}_{i}-\tilde{q}_{j}\right)\right) \tag{5}
\end{equation*}
$$

where the summation in Equation 5 simply loops over all possible two-particle interactions.
Using the definitions assigned in Equation 3, we can, once again, find unitless analogs to $H_{0}$ and $V$, now in four dimensions. Here,

$$
H_{0}=\frac{1}{2} \hbar \omega\left(\boldsymbol{P}^{2}+\boldsymbol{Q}^{2}\right), \text { and }
$$

$$
V=\frac{g}{\sigma}\left(\sum_{i=1}^{4} \sum_{j>i}^{4} \delta\left(q_{i}-q_{j}\right)\right)
$$

where we define $\boldsymbol{P}=\left(p_{1}, p_{2}, p_{3}, p_{4}\right)^{\top}$ and $\boldsymbol{Q}=\left(q_{1}, q_{2}, q_{3}, q_{4}\right)^{\top}$ in the four-particle case.
We can now define the unitless total Hamiltonian in four-dimensions as

$$
\begin{aligned}
H_{g} & =\frac{H_{0}+V}{\hbar \omega} \\
& =\frac{1}{2}\left(\boldsymbol{P}^{2}+\boldsymbol{Q}^{2}\right)+\gamma\left(\sum_{i=1}^{4} \sum_{j>i}^{4} \delta\left(q_{i}-q_{j}\right)\right) .
\end{aligned}
$$

## B. Hamiltonian in Four-Dimensional Jacobi Space

The Jacobi space coordinates can be transformed into Jacobi space coordinates by the rotation matrix

$$
J_{4}=\left(\begin{array}{cccc}
\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 \\
\frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & -\sqrt{\frac{2}{3}} & 0 \\
\frac{1}{2 \sqrt{3}} & \frac{1}{2 \sqrt{3}} & \frac{1}{2 \sqrt{3}} & -\frac{\sqrt{3}}{2} \\
\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2}
\end{array}\right) .
$$

Similar to the transformation in 2- and 3-dimensions, $J_{4} \boldsymbol{Q}=\boldsymbol{R}$ and $J_{4} \boldsymbol{P}=\boldsymbol{K}$. Thus, in four-dimensional Jacobi space, the total, unitless Hamiltonian is

$$
\begin{align*}
H_{g}= & \frac{1}{2}\left(\boldsymbol{K}^{2}+\boldsymbol{R}^{2}\right)+\gamma\left[\delta\left(\sqrt{2} r_{1}\right)\right. \\
& +\delta\left(\frac{1}{\sqrt{2}} r_{1}+\sqrt{\frac{3}{2}} r_{2}\right) \\
& +\delta\left(\frac{1}{\sqrt{2}} r_{1}+\frac{1}{\sqrt{6}} r_{2}+\frac{2}{\sqrt{3}} r_{3}\right) \\
& +\delta\left(-\frac{1}{\sqrt{2}} r_{1}+\sqrt{\frac{3}{2}} r_{2}\right) \\
& +\delta\left(-\frac{1}{\sqrt{2}} r_{1}+\frac{1}{\sqrt{6}} r_{2}+\frac{2}{\sqrt{3}} r_{3}\right) \\
& \left.+\delta\left(-\sqrt{\frac{2}{3}} r_{2}+\frac{2}{\sqrt{3}} r_{3}\right)\right], \tag{6}
\end{align*}
$$

where $\boldsymbol{K}=\left(k_{1}, k_{2}, k_{3}, k_{4}\right)^{\top}$ and $\boldsymbol{R}=\left(r_{1}, r_{2}, r_{3}, r_{4}\right)^{\top}$ in four dimensions.

In the form for $H_{g}$ in Equation 6 we see that the Hamiltonian of four equal-mass harmonic oscillators in one dimension is isomorphic to one isotropic harmonic oscillator in four dimensions [1]. We can also say analogous statements for the two-, three-, and N- particle cases.

## VI. SEPARABILITY

There are two important things to notice about the $r_{4}$, center of mass, coordinate. First, $r_{4}$ is not present in the contact potential component $(V)$ of Equation 6. Second, the $r_{4}$ coordinate separates from $\boldsymbol{r}$ in the trap potential component of Equation 6. This is called separability and is the motivation for the transformation from particle space to Jacobi space.

This separability allows us to express the energy eigenstates "as an unentangled product of center-of-mass and relative wave functions" [1]. The Hamiltonian $H_{g}$ can be written as a sum of the center of mass Hamiltonian $H_{r_{4}}$ and the relative Hamiltonian $H_{r}$. That is,

$$
\begin{aligned}
H_{g} & =\frac{1}{2}\left(\boldsymbol{K}^{2}+\boldsymbol{R}^{2}\right)+V(\boldsymbol{r}) \\
& =\frac{1}{2}\left(\boldsymbol{k}^{2}+k_{4}^{2}+\boldsymbol{r}^{2}+r_{4}^{2}\right)+V(\boldsymbol{r}) \\
& =\frac{1}{2}\left(k_{4}^{2}+r_{4}^{2}\right)+\frac{1}{2}\left(\boldsymbol{k}^{2}+\boldsymbol{r}^{2}\right)+V(\boldsymbol{r}) \\
& =H_{r_{4}}+H_{\boldsymbol{r}}
\end{aligned}
$$

where we've defined $H_{r_{4}}=\frac{1}{2}\left(k_{4}^{2}+r_{4}^{2}\right)$ and $H_{r}=\frac{1}{2}\left(\boldsymbol{k}^{2}+\boldsymbol{r}^{2}\right)+V(\boldsymbol{r})$. In assuming that an eigenstate $\psi(\boldsymbol{R})$ can be written in the form $\psi(\boldsymbol{R})=\psi_{r_{4}}\left(r_{4}\right) \psi_{\boldsymbol{r}}(\boldsymbol{r})$ ), we can write the Schrödinger equation (cf. Equation 8 in Section VII) as

$$
\begin{array}{r}
\left(H_{r_{4}}+H_{\boldsymbol{r}}\right) \psi_{r_{4}}\left(r_{4}\right) \psi_{\boldsymbol{r}}(\boldsymbol{r})=E \psi_{r_{4}}\left(r_{4}\right) \psi_{\boldsymbol{r}}(\boldsymbol{r}) \\
\quad \Rightarrow \frac{H_{r_{4}}\left(\psi_{r_{4}}\left(r_{4}\right)\right)}{\psi_{r_{4}}\left(r_{4}\right)}+\frac{H_{\boldsymbol{r}}\left(\psi_{\boldsymbol{r}}(\boldsymbol{r})\right)}{\psi_{\boldsymbol{r}}(\boldsymbol{r})}=E .
\end{array}
$$

Written in such a way, we see that under the Jacobi transformation the energy eigenstates can be written as an unentangled product of center-of-mass and relative wave functions.

## VII. STATIONARY STATES

For one particle in a one-dimensional harmonic trap, the dynamic equation is given by

$$
\begin{equation*}
i \hbar \frac{\partial \psi}{\partial t}=\hat{H} \psi \tag{7}
\end{equation*}
$$

Our goal is to find the system's stationary states, i.e. our goal is to find the wavefunctions in which $|\psi(x, t)|^{2}=|\psi(x, 0)|^{2}$. This is equivalent to finding the eigenfunctions of the Hamiltonian operator

$$
\begin{equation*}
\hat{H} \psi(x, t)=E \psi(x, t) \tag{8}
\end{equation*}
$$

By finding these stationary states we discover a basis that can be used to describe the nonstationary states. In one dimension with only one particle, this discovery is trivial. There is only one way to distribute any given energy among one particle in one dimension, so the solution of Equation 7 is trivially $\psi(x, t)=e^{-i H_{g} t / \hbar} \psi(x, 0)$.

In four particles in one dimension, finding the stationary states proves more useful. By exploiting the symmetries of the four particles, we will be able to easily calculate the eigenfunctions of the trap Hamiltonian. The stationary states of the trap Hamiltonian form a basis for all square-integrable function on configuration space and we can use these eigenfunctions to approximate the eigenfunctions of the total (i.e., trap and interaction) Hamiltonian.

## VIII. SYMMETRIC GROUP OF FOUR PARTICLES

A group is a collection of transformations of a given point set, which (1) contains the identity transformation; (2) for every transformation $M$, also contains its inverse $M^{-1}$; and (3) includes the composition of all member transformations [13]. One type of group is the symmetric group of four elements $S_{4}$ (not to be confused with the $S_{4}$ rotation-reflection class), which is the group of all permutations on four symbols. With four identical particles in our system there are $4!=24$ possible permutations.

Within the symmetric group of four elements there are five types (or classes) of permutations. Each permutation in a given class is of the same type of particle exchange. A permutation in which no particles are exchanged is in the identity class $E$; a permutation in which three particles are exchanged is in class $C_{3}$; a permutation in which there are two,
two-particle switches is in class $C_{2}$; a permutation in which there is one, two-particle switch is in class $\sigma_{d}$; and a permutation in which all four particles are exchanged is in class $S_{4}$. This class structure is further explained in Section VIIIB.

## A. Configuration Space Representation in the Particle Basis

One representation of the $T_{d}$ group can be found in the particle basis of the four particles. We can build $24,4 \times 4$ matrices to represent the permutations of the group. Defining the row vectors

$$
\begin{align*}
& \boldsymbol{q}_{\mathbf{1}}=(1,0,0,0), \boldsymbol{q}_{\mathbf{2}}=(0,1,0,0) \\
& \boldsymbol{q}_{\boldsymbol{3}}=(0,0,1,0), \text { and } \boldsymbol{q}_{\boldsymbol{4}}=(0,0,0,1), \tag{9}
\end{align*}
$$

we are able to represent each permutation of the four particles as a matrix. The matrix

$$
\left(\begin{array}{l}
\boldsymbol{q}_{1} \\
\boldsymbol{q}_{2} \\
\boldsymbol{q}_{3} \\
\boldsymbol{q}_{4}
\end{array}\right)=\left(\begin{array}{llll}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{array}\right)
$$

for example, represents the identity (the permutation in which no particles are exchanged). The matrix

$$
\left(\begin{array}{l}
\boldsymbol{q}_{\boldsymbol{2}} \\
\boldsymbol{q}_{1} \\
\boldsymbol{q}_{4} \\
\boldsymbol{q}_{3}
\end{array}\right)=\left(\begin{array}{llll}
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0
\end{array}\right)
$$

on the other hand, represents the permutation in which particles 1 and 2 are exchanged and particles 3 and 4 are exchanged. The 24 matrices of this form form a representation of the $T_{d}$ group in particle space. In this representation, each matrix is a representation of a configuration in particle space and will be denoted $M_{i}^{q}$. The operator corresponding to the element $M_{i}^{q}$ in the $T_{d}$ group is denoted $D^{q}\left(M_{i}\right)$. The operator group in configuration space is denoted $D^{q}\left(T_{d}\right)$ and is a representation of the group.

## B. Configuration Space Representation in the Jacobi Cartesian Basis

In the orthonormal Jacobi space (i.e., in the vector space in which $r_{1}, r_{2}, r_{3}$, and $r_{4}$ are orthonormal basis vectors) we can plot the particle space coordinate vectors. Taking any vector in particle space and left-multiplying it by $J_{4}$ yields the particle space coordinate in terms of the Jacobi space coordinates. For example,

$$
J_{4} \cdot \boldsymbol{q}_{1}^{\top}=\frac{1}{\sqrt{2}} \boldsymbol{r}_{1}+\frac{1}{\sqrt{6}} \boldsymbol{r}_{2}+\frac{1}{2 \sqrt{3}} \boldsymbol{r}_{3}+\frac{1}{2} \boldsymbol{r}_{\mathbf{4}}
$$

where $q_{1}^{\top}=(1,0,0,0)^{\top}$ is defined in Equation 9. The conversion is similar for the other particle coordinate vectors.

We truncate the four-dimensional $\boldsymbol{q}_{\mathbf{1}}{ }^{\top}, \boldsymbol{q}_{\mathbf{2}}{ }^{\top}, \boldsymbol{q}_{\boldsymbol{3}}{ }^{\top}$, and $\boldsymbol{q}_{\boldsymbol{4}}{ }^{\top}$ vectors to three dimensions and plot these vectors in the three-dimensional Jacobi space (i.e., the $r_{1}, r_{2}, r_{3}$ orthonormal basis). Truncating the particle space coordinates, equivalent to ignoring the $r_{4}$ coordinate, is justified in Section VI and will be further explained below. A plot of the particle coordinates in the Jacobi basis is shown in Figure 3.


FIG. 3: This figure shows the particle coordinate vectors plotted in the three-dimensional Jacobi space. The fourth dimension is truncated from the particle coordinate vectors and the $r_{4}$ coordinate is ignored entirely. The particle coordinate vectors form the vertices of a regular tetrahedron. The $q_{1}, q_{2}$, and $q_{3}$ vectors are vertically rotated by $\arccos \left(\frac{2 \sqrt{2}}{3}\right)$ radians $(\approx 19.5$ degrees $)$ above the $r_{1}-r_{2}$ plane and the angle between any two $q_{i}$ vectors is arccos $\left(-\frac{1}{3}\right)$ radians ( $\approx 109.5$ degrees).

In Figure 3, the $q_{i}$ particle coordinate vectors form the vertices of a regular tetrahedron in three dimensions. Under the $J_{4}$ Jacobi transformation truncated to three dimensions, the $S_{4}$ symmetric group is arranged as the tetrahedral $T_{d}$ group. In Jacobi space, any permutation that brings the tetrahedron into coincidence with itself is a symmetry element of the $T_{d}$ group.

One possible permutation is the one in which particles 1 and 2 are exchanged and particles 3 and 4 are exchanged (denoted by P2143). This is a rotation of $\pi$ about the vector $(0, \sqrt{2}, 1)^{\top}$ in three dimensions and can be represented by the matrix transformation

$$
J_{4}\left(\begin{array}{llll}
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0
\end{array}\right) J_{4}^{-1}=\left(\begin{array}{cccc}
-1 & 0 & 0 & 0 \\
0 & \frac{1}{3} & \frac{2 \sqrt{2}}{3} & 0 \\
0 & \frac{2 \sqrt{2}}{3} & -\frac{1}{3} & 0 \\
0 & 0 & 0 & 1
\end{array}\right) .
$$

This is one of the three, two-fold rotations that make up the $C_{2}$ class in the $T_{d}$ group.
The 24 elements of the $T_{d}$ group are categorized in 5 classes: the identity $E$; eight, threefold rotations $C_{3}$; three, two-fold rotations $C_{2}$; six mirror reflections $\sigma_{d}$; and six, four-fold rotation-reflections $S_{4}$ [13]. The permutations are characterized by class in Table I. See Appendix A for a table of the 24 permutation matrices written in the Jacobi basis.

| $E(1)$ | $C_{3}(8)$ | $C_{2}(3)$ | $\sigma_{d}(6)$ | $S_{4}(6)$ |
| :---: | :--- | :--- | :--- | :--- |
| $P 1234$ | $P 1342$ | $P 2143$ | $P 1243$ | $P 2341$ |
|  | $P 1423$ | $P 3412$ | $P 1324$ | $P 2413$ |
|  | $P 2314$ | $P 4321$ | $P 1432$ | $P 3142$ |
|  | $P 2431$ |  | $P 2134$ | $P 3421$ |
|  | $P 3124$ |  | $P 3214$ | $P 4123$ |
|  | $P 3241$ |  | $P 4231$ | $P 4312$ |
|  | $P 4132$ |  |  |  |
|  | $P 4213$ |  |  |  |

TABLE I: This table characterizes each permutation as an element in one of the five classes of the $T_{d}$ group. The notation " $P 2431$ " indicates that particle 2 is in the original position of particle 1 , particle 4 is in the original position of particle 2, particle 3 is in its original position, and particle 1 is in the original position of particle 4.

The 24 matrices of this form form a representation of the $T_{d}$ group in Jacobi space. In this representation, each matrix is a representation of a configuration in Jacobi space and will
be denoted $M_{i}^{r}$. The operator corresponding to the element $M_{i}^{r}$ in the $T_{d}$ group is denoted $D^{r}\left(M_{i}\right)$. The operator group in Jacobi space is denoted $D^{r}\left(T_{d}\right)$ and is a representation of the group. Further, the $D^{q}\left(T_{d}\right)$ and $D^{r}\left(T_{d}\right)$ representations are equivalent representations, as they have the same structure and differ only by choice of basis [13].

## C. Hilbert Space Representation in the Jacobi Cartesian Trap Eigenbasis

The first two representations (especially the first) are somewhat trivial. The representation in particle space $D^{q}\left(T_{d}\right)$ is straightforward, and the representation in Jacobi space $D^{r}\left(T_{d}\right)$ is simply a change of basis from the first. In order to construct additional representations we now move from configuration space to the infinite-dimensional Hilbert space - the space of all square-integrable functions. We can take an already-existing transformation and associate with it a linear operator that can act on functions.

Still ignoring the $r_{4}$ coordinate, in the following representations the functions onto which our operators will act will be the harmonic oscillator wavefunctions of three relative particle coordinates in one dimension $\Psi_{n_{1}^{\prime}, n_{2}^{\prime}, n_{3}^{\prime}}\left(r_{1}, r_{2}, r_{3}\right)$. We first define the harmonic oscillator wavefunction of one particle in one dimension as

$$
\begin{equation*}
\psi_{n_{i}^{\prime}}\left(r_{i}\right)=\frac{\pi^{-1 / 4}}{\sqrt{2^{n} n!}}\left(H_{n_{i}^{\prime}}\left(r_{i}\right)\right) e^{-r_{i}^{2} / 2} \tag{10}
\end{equation*}
$$

where $\left(H_{n_{i}^{\prime}}\left(r_{i}\right)\right)$ is the $n_{i}^{\prime}$-th order Hermite polynomial and $n_{i}^{\prime}$ is the energy level of the $i$-th relative coordinate.

In order to expand our definition to three relative particle coordinates in one dimension we simply multiply three of the wavefunctions defined in Equation 10. Thus, our three-particle wavefunction $\Psi_{n_{1}^{\prime}, n_{2}^{\prime}, n_{3}^{\prime}}\left(r_{1}, r_{2}, r_{3}\right)$ is defined as

$$
\begin{equation*}
\Psi_{n_{1}^{\prime}, n_{2}^{\prime}, n_{3}^{\prime}}\left(r_{1}, r_{2}, r_{3}\right)=\psi_{n_{1}^{\prime}}\left(r_{1}\right) \psi_{n_{2}^{\prime}}\left(r_{2}\right) \psi_{n_{3}^{\prime}}\left(r_{3}\right) . \tag{11}
\end{equation*}
$$

Further, in this representation our linear operators will be the permutation matrices in Jacobi space ( $M_{i}^{r}$, or equivalently, $J_{4} M_{i}^{p} J_{4}^{-1}$ ) discussed in Section VIII B.

Having $M_{i}^{r}$ act on $\Psi_{n_{1}^{\prime}, n_{2}^{\prime}, n_{3}^{\prime}}\left(r_{1}, r_{2}, r_{3}\right)$ is equivalent to

$$
\Psi_{n_{1}^{\prime}, n_{2}^{\prime}, n_{3}^{\prime}}\left(M_{i}^{r} \cdot\left(r_{1}, r_{2}, r_{3}\right)\right)=\Psi_{n_{1}^{\prime}, n_{2}^{\prime}, n_{3}^{\prime}}\left(M_{i}^{r} \cdot \boldsymbol{r}\right)
$$

and yields the function

$$
\begin{align*}
& \Psi_{n_{1}^{\prime}, n_{2}^{\prime}, n_{3}^{\prime}}\left(M_{i}^{r} \cdot \boldsymbol{r}\right) \\
& =\left[\psi_{n_{1}^{\prime}}\left(\left[M_{i}^{r} \cdot \boldsymbol{r}\right]_{1}\right) \psi_{n_{2}^{\prime}}\left(\left[M_{i}^{r} \cdot \boldsymbol{r}\right]_{2}\right)\right. \\
& \left.\quad \psi_{n_{3}^{\prime}}\left(\left[M_{i}^{r} \cdot \boldsymbol{r}\right]_{3}\right)\right], \tag{12}
\end{align*}
$$

where $\left[M_{i}^{r} \cdot \boldsymbol{r}\right]_{1}$ is the first element of the $\left(M_{i}^{r} \cdot \boldsymbol{r}\right)$ vector, $\left[M_{i}^{r} \cdot \boldsymbol{r}\right]_{2}$ is the second element, etc.

We are now ready to calculate the wavefunction defined in Equation 12. We begin by calculating the wavefunctions for the unpermuted particles for all possible energy distributions. For total energy $N=n_{1}^{\prime}+n_{2}^{\prime}+n_{3}^{\prime}$ the degeneracy $d_{N}$ (the number of ways to distribute $N$ units of energy among the three relative particle coordinates) is given by

$$
d_{N}=\frac{(N+1)(N+2)}{2} .
$$

For example, with two units of energy $(N=2)$ there are 6 ways to distribute the energy among $r_{1}, r_{2}$, and $r_{3}$; for $N=3$ there are 10 ways; etc. A table of possible distributions for $N=2$ is shown in Table II. In our solution for this representation we calculated wavefunctions for all distributions through $N=3$.

$$
\begin{array}{c|c|c|c|c|c|c}
\boldsymbol{N}=\mathbf{2} & \text { State 1 } & \text { State 2 } & \text { State 3 } & \text { State 4 } & \text { State 5 } & \text { State 6 } \\
\hline\left(n_{1}^{\prime}, n_{2}^{\prime}, n_{3}^{\prime}\right) & (0,0,2) & (0,1,1) & (0,2,0) & (1,0,1) & (1,1,0) & (2,0,0)
\end{array}
$$

TABLE II: This table shows all possible distributions of two units of total energy among $r_{1}, r_{2}$, and $r_{3}$. Each column is a possible distribution state. $n_{i}^{\prime}=0$ indicates that the $i$-th coordinate is in the ground state, $n_{i}^{\prime}=1$ indicates that the $i$-th coordinate is in the first excited state, etc.

Next, we calculated the wavefunctions of each energy distribution in each of the 24 possible permutations. That is, we calculated $\Psi_{n_{1}^{\prime}, n_{2}^{\prime}, n_{3}^{\prime}}\left(M_{i}^{r} \cdot \boldsymbol{r}\right)$ with all possible $M_{i}^{r}$ permutation matrices. If the Hamiltonian $H_{g}$ is invariant under a symmetry transformation $M_{i}^{r}$, then we should be able to use the unpermuted wavefunctions of a given total energy to build a basis with which to write each of the permuted wavefunctions of that total energy [13]. This is equivalent to saying that when the $M_{i}^{r}$ operators act on a permuted wavefunction of a certain energy, the unpermuted wavefunctions of that energy simply "mix" together.

For example, in the $N=2$ family we have six unpermuted wavefunctions that are used
as a basis. We can pick any permuted wavefunction of any $N=2$ energy distribution and write it as a linear combination of the six unpermuted $N=2$ wavefunctions.

Carrying out this procedure for all operators $M_{i}^{r}$ in the $T_{d}$ symmetry group we obtain representations for the $N=0$ state, the $N=1$ states, the $N=2$ states, etc., which together form a representation for the entire group. This Jacobi space representation in a function space basis will be denoted $D^{f}\left(T_{d}\right)$.

## IX. TRANSITION COEFFICIENTS BETWEEN DIFFERENT EIGENBASES OF FUNCTIONS ON CONFIGURATION SPACE

For the four representations that have been constructed thus far we need a method for transforming between different eigenbases of functions on configuration space. $\Psi_{n_{1}^{\prime}, n_{2}^{\prime}, n_{3}^{\prime}, n_{4}^{\prime}}(\boldsymbol{R})$ represents functions with a well defined center-of-mass Jacobi cartesian mode excitation, whereas $\Psi_{n_{1}^{\prime}, n_{2}^{\prime}, n_{3}^{\prime}, n_{4}^{\prime}}\left(J_{4}^{-1} \cdot \boldsymbol{R}\right)$ represents functions with a well defined particle excitation. In this section we derive the transformation matrices to transform one basis to another.

This derivation follows the general procedure just described in Section VIIIC. In this transformation, however, we calculate the wavefunctions untransformed by any operator and use them as a basis to write the wavefunctions transformed by the $J_{4}^{-1}$ operator.

First, we calculate the wavefunctions of the form

$$
\begin{aligned}
& \Psi_{n_{1}^{\prime}, n_{2}^{\prime}, n_{3}^{\prime}, n_{4}^{\prime}}(\boldsymbol{R}) \\
& =\psi_{n_{1}^{\prime}}\left(r_{1}\right) \quad \psi_{n_{2}^{\prime}}\left(r_{2}\right) \psi_{n_{3}^{\prime}}\left(r_{3}\right) \psi_{n_{4}^{\prime}}\left(r_{4}\right)
\end{aligned}
$$

for all possible energy distributions. For total energy $N=n_{1}^{\prime}+n_{2}^{\prime}+n_{3}^{\prime}+n_{4}^{\prime}$ the degeneracy $d_{N}$, now for four relative particle coordinates, is given by

$$
d_{N}=\frac{(N+1)(N+2)(N+3)}{6} .
$$

For example, with two units of energy $(N=2)$ there are now 10 ways to distribute the energy among $r_{1}, r_{2}, r_{3}$, and $r_{4}$; for $N=3$ there are 20 ways; etc. In our solution for the transition coefficients we calculated wavefunctions for all distributions through $N=4$.

Next we calculated the wavefunctions transformed by the $J_{4}^{-1}$ operator. The wavefunctions took the form

$$
\begin{aligned}
& \Psi_{n_{1}^{\prime}, n_{2}^{\prime}, n_{3}^{\prime}, n_{4}^{\prime}}\left(J_{4}^{-1} \cdot \boldsymbol{R}\right) \\
& =\left[\psi_{n_{1}^{\prime}}\left(\left[J_{4}^{-1} \cdot \boldsymbol{R}\right]_{1}\right) \psi_{n_{2}^{\prime}}\left(\left[J_{4}^{-1} \cdot \boldsymbol{R}\right]_{2}\right)\right. \\
& \left.\quad \psi_{n_{3}^{\prime}}\left(\left[J_{4}^{-1} \cdot \boldsymbol{R}\right]_{3}\right) \psi_{n_{4}^{\prime}}\left(\left[J_{4}^{-1} \cdot \boldsymbol{R}\right]_{4}\right)\right]
\end{aligned}
$$

where, as before, $\left[J_{4}^{-1} \cdot \boldsymbol{R}\right]_{1}$ is the first element of the $\left(J_{4}^{-1} \cdot \boldsymbol{R}\right)$ vector, $\left[J_{4}^{-1} \cdot \boldsymbol{R}\right]_{2}$ is the second element, etc.

If the non-interacting Hamiltonian $H_{0}$ is invariant under the $J_{4}^{-1}$ transformation, then we should, once again, be able to use the untransformed wavefunctions of a given total energy to build a basis with which to write each of the transformed wavefunctions of that total energy [13].

Under the $J_{4}^{-1}$ operator we find that we obtain representations for the $N=0$ state, the $N=1$ states, the $N=2$ states, etc., which together form a representation for the entire group, which will be denoted $D_{p}^{f}\left(T_{d}\right)$.

## X. IRREDUCIBLE REPRESENTATIONS: SYSTEMS OF TWO PARTICLES

To construct irreducible representations in our four-particle system we begin by presenting the method in the two-particle case. The two-particle method generalizes to systems of any number of particles.

In our two-particle system, our unitless trap Hamiltonian operator is given by

$$
\hat{H}=\hbar \omega\left(-\frac{\partial^{2}}{\partial q_{1}^{2}}-\frac{\partial^{2}}{\partial q_{2}^{2}}+q_{1}^{2}+q_{2}^{2}\right)
$$

and acts on the two-particle wavefunction

$$
\Psi_{n_{1}, n_{2}}\left(q_{1}, q_{2}\right)=\psi_{n_{1}}\left(q_{1}\right) \psi_{n_{2}}\left(q_{2}\right)
$$

where $\psi_{n_{i}}\left(q_{i}\right)$ is defined as in Equation 10.
In this system there are four types of symmetries, and thus four group elements associated with this Hamiltonian: the identity $E$, the parity transformation $\pi$, the reflection $\sigma$, and the
parity-reflection transformation $\pi \sigma$. We can take these transformations and associate with them linear operators $\hat{U}$ that can act on functions. For $n_{1}=n_{2}$, the effects of these operators leaves each of the wavefunctions unchanged, and for $n_{1} \neq n_{2}$, using the property of Hermite polynomials in which $H_{n_{i}}\left(-q_{i}\right)=(-1)^{n_{i}} H_{n_{i}}\left(q_{i}\right)$, the effects of each of these operators are outlined below.

$$
\begin{align*}
\hat{U}(E) \Psi_{n_{1}, n_{2}}\left(q_{1}, q_{2}\right) & =\Psi_{n_{1}, n_{2}}\left(q_{1}, q_{2}\right) \\
\hat{U}(\pi) \Psi_{n_{1}, n_{2}}\left(q_{1}, q_{2}\right) & =\Psi_{n_{1}, n_{2}}\left(-q_{1},-q_{2}\right) \\
& =(-1)^{n_{1}+n_{2}} \Psi_{n_{1}, n_{2}}\left(q_{1}, q_{2}\right) \\
\hat{U}(\sigma) \Psi_{n_{1}, n_{2}}\left(q_{1}, q_{2}\right) & =\Psi_{n_{1}, n_{2}}\left(q_{2}, q_{1}\right)  \tag{13}\\
& =\Psi_{n_{2}, n_{1}}\left(q_{1}, q_{2}\right) \\
\hat{U}(\pi \sigma) \Psi_{n_{1}, n_{2}}\left(q_{1}, q_{2}\right) & =\Psi_{n_{1}, n_{2}}\left(-q_{2},-q_{1}\right) \\
& =(-1)^{n_{1}+n_{2}} \Psi_{n_{2}, n_{1}}\left(q_{1}, q_{2}\right)
\end{align*}
$$

That is, the identity operator leaves the particle coordinates unchanged, the parity operator reverses the sign of each of the particle coordinates $\left(q_{1} \rightarrow-q_{1}\right.$ and $\left.q_{2} \rightarrow-q_{2}\right)$, the reflection operator switches the particle coordinates $\left(q_{1} \leftrightarrow q_{2}\right)$, and the parity-reflection operator both reverses the signs of and switches the particle coordinates $\left(q_{1} \rightarrow-q_{2}\right.$ and $\left.q_{2} \rightarrow-q_{1}\right)$.

We can represent each of these transformations as matrices by defining $\Psi_{n_{1}, n_{2}}\left(q_{1}, q_{2}\right) \rightarrow$ $(1,0)^{\top}$ and $\Psi_{n_{2}, n_{1}}\left(q_{1}, q_{2}\right) \rightarrow(0,1)^{\top}$. Using these definitions,

$$
\begin{aligned}
& E \rightarrow\left(\begin{array}{ll}
1 & 0 \\
0 & 1
\end{array}\right), \pi \rightarrow\left(\begin{array}{cc}
(-1)^{n_{1}+n_{2}} & 0 \\
0 & (-1)^{n_{1}+n_{2}}
\end{array}\right) \\
& \sigma \rightarrow\left(\begin{array}{ll}
0 & 1 \\
1 & 0
\end{array}\right), \text { and } \pi \sigma \rightarrow\left(\begin{array}{cc}
0 & (-1)^{n_{1}+n_{2}} \\
(-1)^{n_{1}+n_{2}} & 0
\end{array}\right) .
\end{aligned}
$$

The collection of these four matrices is a reducible representation of the group.
In order to break this representation into irreducible representations, we next find any eigenvectors common to all four of these matrices. For both the $e$ and $\pi$ matrices, all vectors
are eigenvectors, and both $\sigma$ and $\pi \sigma$ share the eigenvectors

$$
\binom{\frac{1}{\sqrt{2}}}{\frac{1}{\sqrt{2}}} \text { and }\binom{\frac{1}{\sqrt{2}}}{-\frac{1}{\sqrt{2}}}
$$

which will be denoted $\Psi_{n_{1}, n_{2}}^{+}$and $\Psi_{n_{1}, n_{2}}^{-}$, respectively.
Now, in a method identical to the one shown in Equation 13, we compute the effect of each of the operators on our new eigenvectors. The effects of each of these operators on the two eigenvectors are outlined below.

$$
\begin{aligned}
\hat{U}(E) \Psi_{n_{1}, n_{2}}^{ \pm} & =\Psi_{n_{1}, n_{2}}^{ \pm} \\
\hat{U}(\pi) \Psi_{n_{1}, n_{2}}^{ \pm} & =\frac{1}{\sqrt{2}}\left(\hat{U}(\pi) \Psi_{n_{1}, n_{2}} \pm \hat{U}(\pi) \Psi_{n_{2}, n_{1}}\right) \\
& =(-1)^{n_{1}+n_{2}} \Psi_{n_{1}, n_{2}}^{ \pm} \\
\hat{U}(\sigma) \Psi_{n_{1}, n_{2}}^{ \pm} & =\frac{1}{\sqrt{2}}\left(\hat{U}(\sigma) \Psi_{n_{1}, n_{2}} \pm \hat{U}(\sigma) \Psi_{n_{2}, n_{1}}\right) \\
& = \pm \Psi_{n_{1}, n_{2}}^{ \pm} \\
\hat{U}(\pi \sigma) \Psi_{n_{1}, n_{2}}^{ \pm} & =\frac{1}{\sqrt{2}}\left(\hat{U}(\pi \sigma) \Psi_{n_{1}, n_{2}} \pm \hat{U}(\pi \sigma) \Psi_{n_{2}, n_{1}}\right) \\
& = \pm(-1)^{n_{1}+n_{2}} \Psi_{n_{1}, n_{2}}^{ \pm}
\end{aligned}
$$

We thus have four different types of functions: the $\Psi_{n_{1}, n_{2}}^{+}$functions in which $n_{1}+n_{2}$ is even (the $A_{1}$ representation), the $\Psi_{n_{1}, n_{2}}^{-}$functions in which $n_{1}+n_{2}$ is even (the $A_{2}$ representation), the $\Psi_{n_{1}, n_{2}}^{+}$functions in which $n_{1}+n_{2}$ is odd (the $B_{1}$ representation), and the $\Psi_{n_{1}, n_{2}}^{-}$functions in which $n_{1}+n_{2}$ is odd (the $B_{2}$ representation). Additionally, the wavefunctions for which $n_{1}=n_{2}$ fall into the $A_{1}$ representation.

For example, for $\Psi_{1,0}^{+}$,

$$
\begin{aligned}
& \hat{U}(E) \Psi_{1,0}^{+}=\Psi_{1,0}^{+}, \quad \hat{U}(\pi) \Psi_{1,0}^{+}=-\Psi_{1,0}^{+} \\
& \hat{U}(\sigma) \Psi_{1,0}^{+}=\Psi_{1,0}^{+}, \quad \text { and } \hat{U}(\pi \sigma) \Psi_{1,0}^{+}=-\Psi_{1,0}^{+}
\end{aligned}
$$

and thus $\Psi_{1,0}^{+}$is in the $B_{1}$ representation.
Table III is a character table for the symmetric group of two symbols. The entries in the table are the characters $\chi^{(\mu)}(R)$ (in this case, the $1 \times 1$ matrices) of group element $R$ in irreducible representation $\mu$ for the symmetric group of two elements $S_{2}$.

$$
\begin{array}{|c|cccc||l|}
\hline \mathrm{C}_{2 v} & E(1) & \pi(1) & \sigma(1) & \pi \sigma(1) & \\
\hline A_{1} & 1 & 1 & 1 & 1 & \Psi_{0,0}, \Psi_{1,1}, \Psi_{0,2}^{+}, \Psi_{2,2}, \Psi_{1,3}^{+}, \Psi_{0,4}^{+} \\
A_{2} & 1 & 1 & -1 & -1 & \Psi_{0,2}^{-}, \Psi_{1,3}^{-}, \Psi_{0,4}^{-} \\
B_{1} & 1 & -1 & 1 & -1 & \Psi_{0,1}^{+}, \Psi_{1,2}^{+} \\
B_{2} & 1 & -1 & -1 & 1 & \Psi_{0,1}^{-}, \Psi_{1,2}^{-} \\
\hline
\end{array}
$$

TABLE III: This is the character table for the $\mathrm{C}_{2 v}$ group [13]. The entries in the table are the characters $\chi^{(\mu)}(R)$ (in this case, the $1 \times 1$ matrices) of group element $R$ in irreducible representation $\mu$. In the rightmost column we list the first few wavefunctions in each representation.

| $\mathrm{O}_{h}$ | $E(1)$ | $C_{3}(8)$ | $C_{2}(3)$ | $\sigma_{d}(6)$ | $S_{4}(6)$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $A_{1}$ | 1 | 1 | 1 | 1 | 1 |
| $A_{2}$ | 1 | 1 | 1 | -1 | -1 |
| $E$ | 2 | -1 | 2 | 0 | 0 |
| $F_{2}$ | 3 | 0 | -1 | 1 | -1 |
| $F_{1}$ | 3 | 0 | -1 | -1 | 1 |

TABLE IV: This is the character table for the $\mathrm{O}_{h}$ group [13]. The entries in the table are the characters $\chi^{(\mu)}(R)$ of a group element $R$ in irreducible representation $\mu$.

## XI. PROJECTION ONTO IRREDUCIBLE REPRESENTATIONS

The following projection operator formula encompasses the procedure just outlined in Section X. The projection $P$ of a state onto representation $\mu$ is given by

$$
\begin{equation*}
P^{(\mu)}=\frac{n_{\mu}}{g} \sum_{R}\left(\chi^{(\mu)}(R) M_{R}\right), \tag{14}
\end{equation*}
$$

where $n_{\mu}$ is the dimension of the representation, $g$ is the number of elements in the group, $\chi^{(\mu)}(R)$ is the character of a group element $R$ in representation $\mu$, and $M_{R}$ is the matrix operator for group element $R$ [13].

The character $\chi^{(\mu)}(R)$ of a group element $R$ is simply the trace of a class's permutation matrix in irreducible representation $\mu$ (Table IV). The character is independent of choice of basis [13]. The dimension of the irreducible representation $n_{\mu}$ is the character of the identity element in representation $\mu$.

In the four-particle case, $g=24$, and the summation sums over all 24 of the permutation matrices (truncated to three dimensions) in the Jacobi basis representation.

We can project any wavefunction onto any representation. For example, the projections
of

$$
\Psi_{2,0,0}\left(r_{1}, r_{2}, r_{3}\right)=\frac{e^{\frac{1}{2}\left(-r_{1}^{2}-r_{2}^{2}-r_{3}^{2}\right)}}{\pi^{3 / 4}} \frac{\left(-1+2 r_{1}^{2}\right)}{\sqrt{2}}
$$

onto the five representations are shown in Equation 15.

$$
\begin{align*}
P^{\left(A_{1}\right)} \Psi_{2,0,0} & =\frac{e^{\frac{1}{2}\left(-r_{1}^{2}-r_{2}^{2}-r_{3}^{2}\right)}}{\pi^{3 / 4}} \frac{-3+2 r_{1}^{2}+2 r_{2}^{2}+2 r_{3}^{2}}{3 \sqrt{2}} \\
P^{\left(A_{2}\right)} \Psi_{2,0,0} & =0 \\
P^{(E)} \Psi_{2,0,0} & =\frac{e^{\frac{1}{2}\left(-r_{1}^{2}-r_{2}^{2}-r_{3}^{2}\right)}}{\pi^{3 / 4}} \frac{r_{1}^{2}-r_{2}^{2}-2 \sqrt{2} r_{2} r_{3}}{3 \sqrt{2}}  \tag{15}\\
P^{\left(F_{2}\right)} \Psi_{2,0,0} & =\frac{e^{\frac{1}{2}\left(-r_{1}^{2}-r_{2}^{2}-r_{3}^{2}\right)}}{\pi^{3 / 4}} \frac{3 r_{1}^{2}-r_{2}^{2}+2 \sqrt{2} r_{2} r_{3}-2 r_{3}^{2}}{3 \sqrt{2}} \\
P^{\left(F_{1}\right)} \Psi_{2,0,0} & =0
\end{align*}
$$

If we convert our wavefunctions back to particle coordinates, we find that all projections onto the $A_{1}$ representation are symmetric under all two-particle exchanges, and all projections on the the $A_{2}$ representation are antisymmetric under all two-particle exchanges. Thus, the $A_{1}$ representation is comprised of all-boson systems, and the $A_{2}$ representation is comprised of all-fermion systems. The $E, F_{2}$, and $F_{1}$ representations contain mixtures of distinguishable and indistinguishable particles. Since only the $A_{1}$ and $A_{2}$ representations are comprised of indistinguishable particles, we focus only on these two representations for the remainder of this paper. The method, however, generalizes to any representation.

Additionally, there are no non-zero $A_{2}$ projections for $N<6$, as $N=6$ is the smallest non-negative integer that can be written as a sum of four distinct non-negative integers. This is expected, since the $A_{2}$ representation is the all-fermion representation, for which no two particles in the four-particle system can have the same excitation.

## A. Normalized Projection, Method I

The projected wavefunctions will, in general, not be normalized. To normalize a projected wavefunction we find the normalization constant $A$ such that

$$
\begin{equation*}
\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty}\left(A \Psi_{n_{1}^{\prime}, n_{2}^{\prime}, n_{3}^{\prime}}\right)^{*}\left(A\left(P^{(\mu)} \Psi_{n_{1}^{\prime}, n_{2}^{\prime}, n_{3}^{\prime}}\right)\right) \mathrm{d} r_{1} \mathrm{~d} r_{2} \mathrm{~d} r_{3}=1 . \tag{16}
\end{equation*}
$$

Since all of our irreducible representations are real (or can be brought to real form) [13], Equation 16 simplifies to

$$
\begin{equation*}
A^{2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \Psi_{n_{1}^{\prime}, n_{2}^{\prime}, n_{3}^{\prime}}\left(P^{(\mu)} \Psi_{n_{1}^{\prime}, n_{2}^{\prime}, n_{3}^{\prime}}\right) \mathrm{d} r_{1} \mathrm{~d} r_{2} \mathrm{~d} r_{3}=1 \tag{17}
\end{equation*}
$$

where we've both removed the complex conjugate and factored $A^{2}$ from the integral. In Equation 17's simplified form, evaluating this integral using Mathematica's Integrate function is much more computationally efficient. For the $N=4$ projections, for example, finding the normalization constants via Equation 16 took about 50 minutes, and via Equation 17 took only 30 seconds.

Thus, for non-zero projections,

$$
\begin{equation*}
A=\frac{1}{\sqrt{\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \Psi_{n_{1}^{\prime}, n_{2}^{\prime}, n_{3}^{\prime}}\left(P^{(\mu)} \Psi_{n_{1}^{\prime}, n_{2}^{\prime}, n_{3}^{\prime}}\right) \mathrm{d} r_{1} \mathrm{~d} r_{2} \mathrm{~d} r_{3}}} \tag{18}
\end{equation*}
$$

and our now-normalized, projected wavefunctions $\left(\hat{P}^{(\mu)} \Psi_{n_{1}^{\prime}, n_{2}^{\prime}, n_{3}^{\prime}}\right)$ are given by

$$
\left(\hat{P}^{(\mu)} \Psi_{n_{1}^{\prime}, n_{2}^{\prime}, n_{3}^{\prime}}\right)=A\left(P^{(\mu)} \Psi_{n_{1}^{\prime}, n_{2}^{\prime}, n_{3}^{\prime}}\right),
$$

with $A$ given by Equation 18 .
The normalized $\Psi_{2,0,0}\left(r_{1}, r_{2}, r_{3}\right)$ projections are thus

$$
\begin{aligned}
\hat{P}^{\left(A_{1}\right)} \Psi_{2,0,0} & =\sqrt{3} \frac{e^{\frac{1}{2}\left(-r_{1}^{2}-r_{2}^{2}-r_{3}^{2}\right)}}{\pi^{3 / 4}} \frac{-3+2 r_{1}^{2}+2 r_{2}^{2}+2 r_{3}^{2}}{3 \sqrt{2}} \\
\hat{P}^{\left(A_{2}\right)} \Psi_{2,0,0} & =0 \\
\hat{P}^{(E)} \Psi_{2,0,0} & =\sqrt{6} \frac{e^{\frac{1}{2}\left(-r_{1}^{2}-r_{2}^{2}-r_{3}^{2}\right)}}{\pi^{3 / 4}} \frac{r_{1}^{2}-r_{2}^{2}-2 \sqrt{2} r_{2} r_{3}}{3 \sqrt{2}} \\
\hat{P}^{\left(F_{2}\right)} \Psi_{2,0,0} & =\sqrt{2} \frac{e^{\frac{1}{2}\left(-r_{1}^{2}-r_{2}^{2}-r_{3}^{2}\right)}}{\pi^{3 / 4}} \frac{3 r_{1}^{2}-r_{2}^{2}+2 \sqrt{2} r_{2} r_{3}-2 r_{3}^{2}}{3 \sqrt{2}} \\
\hat{P}^{\left(F_{1}\right)} \Psi_{2,0,0} & =0 .
\end{aligned}
$$

## B. Normalized Projection, Method II

We now propose an alternate, more computationally efficient method for finding the normalized, projected wavefunctions. Instead of using Mathematica's Integrate function, we use the PolynomialReduce, Eigensystem, and Orthogonalize functions.

We begin by calculating all of the wavefunctions of total energy $N$ via Equation 11. To calculate these wavefunctions' normalized projections onto representation $\mu$, we first calculate the unnormalized projections via Equation 14.

Next, we build the matrix representation of the projected wavefunctions of total energy $N$ onto representation $\mu$. Using PolynomialReduce we write the projected wavefunctions $P^{(\mu)} \Psi_{N}$ in terms of the unprojected wavefunctions of the same energy $\Psi_{N}$.

For example, for $N=3$ and $\mu=A_{1}$, we write each of the $P^{\left(A_{1}\right)} \Psi_{N=3}$ 's as a linear combination of the $10 \Psi_{N=3}$ 's. For example,

$$
\begin{aligned}
P^{\left(A_{1}\right)} \Psi_{0,0,3}= & \frac{2}{9} \Psi_{0,0,3}+0 \Psi_{0,1,2}-\frac{1}{3 \sqrt{3}} \Psi_{0,2,1}+\frac{\sqrt{2}}{9} \Psi_{0,3,0}+0 \Psi_{1,0,2} \\
& +0 \Psi_{1,1,1}+0 \Psi_{1,2,0}-\frac{1}{3 \sqrt{3}} \Psi_{2,0,1}-\frac{\sqrt{\frac{2}{3}}}{3} \Psi_{2,1,0}+0 \Psi_{3,0,0}
\end{aligned}
$$

The coefficients on each of these 10 terms form the first row of the matrix. The second row of the matrix is formed by the coefficients on the $\Psi_{N=3}$ 's for $P^{\left(A_{1}\right)} \Psi_{0,1,2}$, the third row is formed by the coefficients on the $\Psi_{N=3}$ 's for $P^{\left(A_{1}\right)} \Psi_{0,2,1}$, etc.

Next, using Eigensystem, we find the eigenvalues and eigenvectors of the coefficient matrix. Using only the eigenvectors with an eigenvalue of 1 (i.e., vectors unchanged by the projection operator), we build an orthonormal basis via the Orthogonalize function. To convert our basis vectors to basis functions, we simply take the dot product of each basis vector with the vector with elements given by the $\Psi_{N}$ 's. The resulting basis function is the normalized projection of all of the nonzero $P^{(\mu)} \Psi_{N}$.

In the $N=3, \mu=A_{1}$ example we find the single basis vector

$$
\left(\begin{array}{lllllllll}
-\frac{\sqrt{2}}{3} & 0 & \frac{1}{\sqrt{6}} & -\frac{1}{3} & 0 & 0 & 0 & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{3}}
\end{array}\right)^{\top}
$$

|  | $N=0$ | $N=1$ | $N=2$ | $N=3$ | $N=4$ | $N=5$ | $N=6$ | $N=7$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $A_{1}$ | 1 | 0 | 1 | 1 | 2 | 1 | 3 | 2 |
| $A_{2}$ | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 |
| $E$ | 0 | 0 | 1 | 0 | 2 | 1 | 3 | 2 |
| $F_{2}$ | 0 | 1 | 1 | 2 | 2 | 4 | 4 | 6 |
| $F_{1}$ | 0 | 0 | 0 | 1 | 1 | 2 | 2 | 4 |

TABLE V: This table shows how many copies of each representation exist for each energy level. The $A_{1}$ and $A_{2}$ representations are one-dimensional, the $E$ representation is two-dimensional, and the $F_{2}$ and $F_{1}$ representations are three-dimensional. To calculate the number of basis functions for a given entry, simply multiply the entry by the dimension of the representation. For example, for $N=5$ and $\mu=F_{2}$ (a three-dimensional representation) there are $4 \times 3=12$ basis functions.

Taking the dot product of this basis vector with

$$
\left(\begin{array}{llllllllll}
\Psi_{0,0,3} & \Psi_{0,1,2} & \Psi_{0,2,1} & \Psi_{0,3,0} & \Psi_{1,0,2} & \Psi_{1,1,1} & \Psi_{1,2,0} & \Psi_{2,0,1} & \Psi_{2,1,0} & \Psi_{3,0,0}
\end{array}\right)^{\top}
$$

yields the basis function

$$
\frac{e^{\frac{1}{2}\left(-r_{1}^{2}-r_{2}^{2}-r_{3}^{2}\right)}}{\pi^{3 / 4}} \frac{\left(6 r_{1}^{2} r_{2}+\sqrt{2} r_{3}\left(3 r_{1}^{2}-2 r_{3}^{2}\right)-2 r_{2}^{3}+3 \sqrt{2} r_{2}^{2} r_{3}\right)}{3 \sqrt{3}}
$$

which is the normalized, projected wavefunction for all nonzero, $N=3$ projections in the $A_{1}$ representation.

For many $N-\mu$ combinations there may be multiple basis functions, in which case the projected wavefunctions are simply a linear combination of the common, orthogonal wavefunctions. In the $N=4$ projection onto the $A_{1}$ representation, for example, all of the projected wavefunctions are some linear combination of two orthogonal wavefunctions.

In our solution, we computed the basis vectors through $N=7$. In Table V we list how many copies of each representation exist for energy levels $N=0$ through $N=7$, and in Appendix B we note the representations and energy levels for which a projected wavefunction is nonzero.

## XII. PARTICLE CLUSTERING

In the orthonormal Jacobi space basis we can find locations describing two separate twoparticle clusters ("2-2 clusters") (in one dimension in Figure 4) and the locations describing
a three particle cluster with one particle on its own ("3-1 clusters") (in one dimension in Figure 5).


FIG. 4: This figure shows an example of a 2-2 particle cluster in which particles $q_{1}$ and $q_{4}$ are in one cluster and particles $q_{2}$ and $q_{3}$ are in another cluster.


FIG. 5: This figure shows an example of a 3-1 particle cluster in which particles $q_{1}, q_{2}$, and $q_{3}$ are in one cluster and particle $q_{4}$ is on its own.

In the orthonormal Jacobi space basis, a plane spanned by any two of the particlecoordinate vectors is a region in which the other two particles are clustered together. For example, the plane spanning the $q_{1}-q_{2}$ vectors is a region in which particles $q_{3}$ and $q_{4}$ are in the same location (Figure 6). There are six planes of this type - one for each two-particle pair. The six planes are shown in Figure 7.


FIG. 6: This figure shows the plane in which particles $q_{3}$ and $q_{4}$ are in the same location. This plane spans the $q_{1}$ and $q_{2}$ vectors, bisecting the angle between particles $q_{3}$ and $q_{4}$. There are 6 planes of this type.


FIG. 7: This figure shows all two-particle clustering planes. Where two planes intersect in a line there is a 2-2 particle clustering, and where three planes intersect in a line there is a $3-1$ particle clustering.

Locations in which two planes intersect in a line are 2-2 particle clusterings, and locations in which three planes intersect in a line are 3-1 particle clusterings. The clustering lines are shown in Figure 8.

We can also describe 1-2-1 particle clusterings (i.e., configurations in which one particle is to the left of a 2-particle cluster and another particle is equidistant to the right of the 2-particle cluster). Not shown in Figure 8, each of the 1-2-1 clustering lines is perpendicular to one of the planes in Figure 7.

## XIII. PROJECTIONS AND PARTICLE CLUSTERING

By overlaying the clustering lines (from Figure 8) with the projected wavefunctions, we notice some interesting results. We first convert our projected wavefunctions to spherical coordinates $\left(r_{1} \rightarrow \rho \sin (\theta) \cos (\phi), r_{2} \rightarrow \rho \sin (\theta) \sin (\phi)\right.$, and $\left.r_{3} \rightarrow \rho \cos (\theta)\right)$ and plot the projected wavefunction at a specified value of $\rho$, effectively plotting only the angular portion of the wavefunction.

In Figure 9 we plot the all-boson $\hat{P}^{\left(A_{1}\right)} \Psi_{4,0,0}$ wavefunction. For this state, there are primary maxima at 2-2 clustering lines and secondary maxima at 3-1 clustering lines. This


FIG. 8: This figure shows all 2-2 and 3-1 clustering lines. The four, 3-1 clustering lines (in red) run along the particle coordinate axes, and the three, 2-2 clustering lines (in blue) bisect the angle between each pair of particle coordinate axes.
preference to clustering is consistent with all wavefunctions in the $A_{1}$ representation. Additionally, one indication that there are multiple copies of the $A_{1}$ representation for $N=4$ is that the relative size of the angular nodes is dependent on our defined value of $\rho$.


FIG. 9: This figure shows the same clustering lines as in Figure 8, overlaid with the projection of $\Psi_{4,0,0}$ onto the $A_{1}$ representation. Note the primary maxima at 2-2 clustering lines and secondary maxima at 3-1 clustering lines for this state.

In Figure 10 we plot the all-fermion $\hat{P}^{\left(A_{2}\right)} \Psi_{3,0,3}$ wavefunction. For this state, there is 0 probability that the particles will cluster in any of the possible formations (i.e., 2-2 clusterings, 3-1 clusterings, and 1-2-1 clusterings). This behavior is consistent with all wavefunctions in the $A_{2}$ representation.


FIG. 10: This figure shows the same clustering lines as in Figure 8, overlaid with the projection of $\Psi_{3,0,3}$ onto the $A_{2}$ representation. Note the 0 probability that the all-fermion state will cluster in any of the possible formations (i.e., 2-2 clusterings, 3-1 clusterings, and 1-2-1 clusterings).

## XIV. CONCLUDING REMARKS

The method we've proposed generalizes nicely to $N$ particles in $d$ dimensions. Using the Jacobi transformation to move from particle coordinates to relative coordinates as described in Section V , we can effectively reduce our problem from one of $(N * d)$ generalized coordinates to $(N * d)-1$. Extensions to $(N * d) \geq 5$ "require using the less-familiar point groups in higher dimensions, which have been classified by Coxeter and others" [1]. For $(N * d) \geq 5$ the problem increases in difficulty, but is still solvable via our method, nonetheless. Additionally, our method for finding the normalized projections described in Section XIB will be of great value for large $(N * d)$. Even in our computation of $(N * d)=4$, this alternate method proves to be more efficient than the standard normalization procedure by evaluation of the three, infinite integrals. Finally, our method for classifying particle clustering described in Section XII and implemented in Section XIII will be of great use in systems of interacting particles.

## Appendix A: Permutation Matrices in the Jacobi Cartesian Basis

In this appendix we list, in the Jacobi basis, the 24 possible permutation matrices. The notation used here is equivalent to the that used in Table I.

1. $E(1)$
$P 1234=\left(\begin{array}{llll}1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1\end{array}\right)$.
2. $C_{3}(8)$
$P 1342=\left(\begin{array}{cccc}\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 & 0 \\ \frac{1}{2 \sqrt{3}} & -\frac{1}{6} & \frac{2 \sqrt{2}}{3} & 0 \\ \sqrt{\frac{2}{3}} & -\frac{\sqrt{2}}{3} & -\frac{1}{3} & 0 \\ 0 & 0 & 0 & 1\end{array}\right), P 1423=\left(\begin{array}{cccc}\frac{1}{2} & \frac{1}{2 \sqrt{3}} & \sqrt{\frac{2}{3}} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{6} & -\frac{\sqrt{2}}{3} & 0 \\ 0 & \frac{2 \sqrt{2}}{3} & -\frac{1}{3} & 0 \\ 0 & 0 & 0 & 1\end{array}\right), P 2314=\left(\begin{array}{cccc}-\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1\end{array}\right)$,
$P 2431=\left(\begin{array}{cccc}-\frac{1}{2} & \frac{1}{2 \sqrt{3}} & \sqrt{\frac{2}{3}} & 0 \\ -\frac{1}{2 \sqrt{3}} & \frac{5}{6} & -\frac{\sqrt{2}}{3} & 0 \\ -\sqrt{\frac{2}{3}} & -\frac{\sqrt{2}}{3} & -\frac{1}{3} & 0 \\ 0 & 0 & 0 & 1\end{array}\right), P 3124=\left(\begin{array}{cccc}-\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1\end{array}\right), P 3241=\left(\begin{array}{cccc}\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 & 0 \\ -\frac{1}{2 \sqrt{3}} & -\frac{1}{6} & \frac{2 \sqrt{2}}{3} & 0 \\ -\sqrt{\frac{2}{3}} & -\frac{\sqrt{2}}{3} & -\frac{1}{3} & 0 \\ 0 & 0 & 0 & 1\end{array}\right)$,
$P 4132=\left(\begin{array}{cccc}-\frac{1}{2} & -\frac{1}{2 \sqrt{3}} & -\sqrt{\frac{2}{3}} & 0 \\ \frac{1}{2 \sqrt{3}} & \frac{5}{6} & -\frac{\sqrt{2}}{3} & 0 \\ \sqrt{\frac{2}{3}} & -\frac{\sqrt{2}}{3} & -\frac{1}{3} & 0 \\ 0 & 0 & 0 & 1\end{array}\right), P 4213=\left(\begin{array}{cccc}\frac{1}{2} & -\frac{1}{2 \sqrt{3}} & -\sqrt{\frac{2}{3}} & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{6} & -\frac{\sqrt{2}}{3} & 0 \\ 0 & \frac{2 \sqrt{2}}{3} & -\frac{1}{3} & 0 \\ 0 & 0 & 0 & 1\end{array}\right)$.
3. $C_{2}(3)$
$P 2143=\left(\begin{array}{cccc}-1 & 0 & 0 & 0 \\ 0 & \frac{1}{3} & \frac{2 \sqrt{2}}{3} & 0 \\ 0 & \frac{2 \sqrt{2}}{3} & -\frac{1}{3} & 0 \\ 0 & 0 & 0 & 1\end{array}\right), P 3412=\left(\begin{array}{cccc}0 & -\frac{1}{\sqrt{3}} & \sqrt{\frac{2}{3}} & 0 \\ -\frac{1}{\sqrt{3}} & -\frac{2}{3} & -\frac{\sqrt{2}}{3} & 0 \\ \sqrt{\frac{2}{3}} & -\frac{\sqrt{2}}{3} & -\frac{1}{3} & 0 \\ 0 & 0 & 0 & 1\end{array}\right)$,
$P 4321=\left(\begin{array}{cccc}0 & \frac{1}{\sqrt{3}} & -\sqrt{\frac{2}{3}} & 0 \\ \frac{1}{\sqrt{3}} & -\frac{2}{3} & -\frac{\sqrt{2}}{3} & 0 \\ -\sqrt{\frac{2}{3}} & -\frac{\sqrt{2}}{3} & -\frac{1}{3} & 0 \\ 0 & 0 & 0 & 1\end{array}\right)$.
4. $\sigma_{d}(6)$
$P 1243=\left(\begin{array}{cccc}1 & 0 & 0 & 0 \\ 0 & \frac{1}{3} & \frac{2 \sqrt{2}}{3} & 0 \\ 0 & \frac{2 \sqrt{2}}{3} & -\frac{1}{3} & 0 \\ 0 & 0 & 0 & 1\end{array}\right), P 1324=\left(\begin{array}{cccc}\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1\end{array}\right), P 1432=\left(\begin{array}{cccc}-1 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2 \sqrt{3}} & \sqrt{\frac{2}{3}} & 0 \\ \frac{1}{2 \sqrt{3}} & \frac{5}{6} & -\frac{\sqrt{2}}{3} & 0 \\ \sqrt{\frac{2}{3}} & -\frac{\sqrt{2}}{3} & -\frac{1}{3} & 0 \\ 0 & 0 & 0 & 1\end{array}\right)$,
$P 2134=\left(\begin{array}{cccc}\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1\end{array}\right), P 4231=\left(\begin{array}{ccc}\frac{1}{2} & -\frac{1}{2 \sqrt{3}} & -\sqrt{\frac{2}{3}} \\ 0\end{array}\right), P 3214=\left(\begin{array}{ccc}-\frac{1}{2 \sqrt{3}} & \frac{5}{6} & -\frac{\sqrt{2}}{3} \\ -\sqrt{\frac{2}{3}} & -\frac{\sqrt{2}}{3} & -\frac{1}{3} \\ 0 \\ 0 & 0 & 0\end{array}\right)$.
5. $S_{4}(6)$

$$
\begin{aligned}
& P 2341=\left(\begin{array}{cccc}
-\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 & 0 \\
-\frac{1}{2 \sqrt{3}} & -\frac{1}{6} & \frac{2 \sqrt{2}}{3} & 0 \\
-\sqrt{\frac{2}{3}} & -\frac{\sqrt{2}}{3} & -\frac{1}{3} & 0 \\
0 & 0 & 0 & 1
\end{array}\right), P 2413=\left(\begin{array}{cccc}
-\frac{1}{2} & \frac{1}{2 \sqrt{3}} & \sqrt{\frac{2}{3}} & 0 \\
-\frac{\sqrt{3}}{2} & -\frac{1}{6} & -\frac{\sqrt{2}}{3} & 0 \\
0 & \frac{2 \sqrt{2}}{3} & -\frac{1}{3} & 0 \\
0 & 0 & 0 & 1
\end{array}\right), P 3142=\left(\begin{array}{cccc}
-\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 & 0 \\
\frac{1}{2 \sqrt{3}} & -\frac{1}{6} & \frac{2 \sqrt{2}}{3} & 0 \\
\sqrt{\frac{2}{3}} & -\frac{\sqrt{2}}{3} & -\frac{1}{3} & 0 \\
0 & 0 & 0 & 1
\end{array}\right), \\
& P 3421=\left(\begin{array}{cccc}
0 & -\frac{1}{\sqrt{3}} & \sqrt{\frac{2}{3}} & 0 \\
\frac{1}{\sqrt{3}} & -\frac{2}{3} & -\frac{\sqrt{2}}{3} & 0 \\
-\sqrt{\frac{2}{3}} & -\frac{\sqrt{2}}{3} & -\frac{1}{3} & 0 \\
0 & 0 & 0 & 1
\end{array}\right), P 4123=\left(\begin{array}{cccc}
-\frac{1}{2} & -\frac{1}{2 \sqrt{3}} & -\sqrt{\frac{2}{3}} & 0 \\
\frac{\sqrt{3}}{2} & -\frac{1}{6} & -\frac{\sqrt{2}}{3} & 0 \\
0 & \frac{2 \sqrt{2}}{3} & -\frac{1}{3} & 0 \\
0 & 0 & 0 & 1
\end{array}\right), \\
& P 4312=\left(\begin{array}{cccc}
0 & \frac{1}{\sqrt{3}} & -\sqrt{\frac{2}{3}} & 0 \\
-\frac{1}{\sqrt{3}} & -\frac{2}{3} & -\frac{\sqrt{2}}{3} & 0 \\
\sqrt{\frac{2}{3}} & -\frac{\sqrt{2}}{3} & -\frac{1}{3} & 0 \\
0 & 0 & 0 & 1
\end{array}\right) .
\end{aligned}
$$

## Appendix B: Nonzero Projections of $\Psi_{n_{1}^{\prime}, n_{2}^{\prime}, n_{3}^{\prime}}\left(r_{1}, r_{2}, r_{3}\right)$

In this appendix we indicate the representations onto which the projections of $\Psi_{n_{1}^{\prime}, n_{2}^{\prime}, n_{3}^{\prime}}$ are nonzero. A $\checkmark$ indicates that there exists at least one copy of a representation for a given wavefunction. See Table $V$ for the number of copies of each representation for each energy.

| $\boldsymbol{N}=\mathbf{0}$ | $A_{1}$ | $A_{2}$ | $E$ | $F_{2}$ | $F_{1}$ |  |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\Psi_{0,0,0}$ | $\checkmark$ |  |  |  |  |  |$\quad$| $\boldsymbol{N}=\mathbf{1}$ | $A_{1}$ | $A_{2}$ | $E$ | $F_{2}$ | $F_{1}$ |
| :--- | :--- | :--- | :--- | :--- | :--- |
| $\Psi_{0,0,1}$ |  |  |  | $\checkmark$ |  |
| $\Psi_{0,1,0}$ |  |  |  |  | $\checkmark$ |
| $\Psi_{1,0,0}$ |  |  |  |  |  |


| $\boldsymbol{N = 2}$ | $A_{1}$ | $A_{2}$ | $E$ | $F_{2}$ | $F_{1}$ |
| :--- | :--- | :--- | :--- | :--- | :--- |
| $\Psi_{0,0,2}$ | $\checkmark$ |  |  | $\checkmark$ |  |
| $\Psi_{0,1,1}$ |  |  | $\checkmark$ | $\checkmark$ |  |
| $\Psi_{0,2,0}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ |  |
| $\Psi_{1,0,1}$ |  |  | $\checkmark$ | $\checkmark$ |  |
| $\Psi_{1,1,0}$ |  |  | $\checkmark$ | $\checkmark$ |  |
| $\Psi_{2,0,0}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ |  |


| $\boldsymbol{N}=\mathbf{3}$ | $A_{1}$ | $A_{2}$ | $E$ | $F_{2}$ | $F_{1}$ |
| :--- | :--- | :--- | :--- | :--- | :--- |
| $\Psi_{0,0,3}$ | $\checkmark$ |  |  | $\checkmark$ |  |
| $\Psi_{0,1,2}$ |  |  |  | $\checkmark$ | $\checkmark$ |
| $\Psi_{0,2,1}$ | $\checkmark$ |  |  | $\checkmark$ | $\checkmark$ |
| $\Psi_{0,3,0}$ | $\checkmark$ |  |  | $\checkmark$ | $\checkmark$ |
| $\Psi_{1,0,2}$ |  |  |  | $\checkmark$ | $\checkmark$ |
| $\Psi_{1,1,1}$ |  |  |  | $\checkmark$ | $\checkmark$ |
| $\Psi_{1,2,0}$ |  |  |  | $\checkmark$ | $\checkmark$ |
| $\Psi_{2,0,1}$ | $\checkmark$ |  |  | $\checkmark$ | $\checkmark$ |
| $\Psi_{2,1,0}$ | $\checkmark$ |  |  | $\checkmark$ | $\checkmark$ |
| $\Psi_{3,0,0}$ |  |  |  | $\checkmark$ | $\checkmark$ |


| $\boldsymbol{N}=\mathbf{4}$ | $A_{1}$ | $A_{2}$ | $E$ | $F_{2}$ | $F_{1}$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $\Psi_{0,0,4}$ | $\checkmark$ |  |  | $\checkmark$ |  |
| $\Psi_{0,1,3}$ |  |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{0,2,2}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{0,3,1}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{0,4,0}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{1,0,3}$ |  |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{1,1,2}$ |  |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{1,2,1}$ |  |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{1,3,0}$ |  |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{2,0,2}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{2,1,1}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{2,2,0}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{3,0,1}$ |  |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{3,1,0}$ |  |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{4,0,0}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ |  |


| $\boldsymbol{N = \mathbf { 5 }}$ | $A_{1}$ | $A_{2}$ | $E$ | $F_{2}$ | $F_{1}$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $\Psi_{0,0,5}$ | $\checkmark$ |  |  | $\checkmark$ |  |
| $\Psi_{0,1,4}$ |  |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{0,2,3}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{0,3,2}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{0,4,1}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{0,5,0}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{1,0,4}$ |  |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{1,1,3}$ |  |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{1,2,2}$ |  |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{1,3,1}$ |  |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{1,4,0}$ |  |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{2,0,3}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{2,1,2}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{2,2,1}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{2,3,0}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{3,0,2}$ |  |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{3,1,1}$ |  |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{3,2,0}$ |  |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{4,0,1}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{4,1,0}$ | $\checkmark$ | $\checkmark$ | $\checkmark$ | $\checkmark$ |  |
| $\Psi_{5,0,0}$ |  |  |  | $\checkmark$ | $\checkmark$ |


| $\boldsymbol{N = 6}$ | $A_{1}$ | $A_{2}$ | $E$ | $F_{2}$ | $F_{1}$ |
| :--- | :--- | :--- | :--- | :--- | :--- |
| $\Psi_{0,0,6}$ | $\checkmark$ |  |  | $\checkmark$ |  |
| $\Psi_{0,1,5}$ |  |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{0,2,4}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{0,3,3}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{0,4,2}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{0,5,1}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{0,6,0}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{1,0,5}$ |  |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{1,1,4}$ |  |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{1,2,3}$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{1,3,2}$ |  |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{1,4,1}$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{1,5,0}$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{2,0,4}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{2,1,3}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{2,2,2}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{2,3,1}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{2,4,0}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{3,0,3}$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{3,1,2}$ |  |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{3,2,1}$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{3,3,0}$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{4,0,2}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{4,1,1}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{4,2,0}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{5,0,1}$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{5,1,0}$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{6,0,0}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ |  |


| $\boldsymbol{N = \mathbf { 7 }}$ | $A_{1}$ | $A_{2}$ | $E$ | $F_{2}$ | $F_{1}$ |
| :--- | :--- | :--- | :--- | :--- | :--- |
| $\Psi_{0,0,7}$ | $\checkmark$ |  |  | $\checkmark$ |  |
| $\Psi_{0,1,6}$ |  |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{0,2,5}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{0,3,4}$ | $\checkmark$ | $\checkmark$ | $\checkmark$ | $\checkmark$ |  |
| $\Psi_{0,4,3}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{0,5,2}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{0,6,1}$ | $\checkmark$ | $\checkmark$ | $\checkmark$ | $\checkmark$ |  |
| $\Psi_{0,7,0}$ | $\checkmark$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |
| $\Psi_{1,0,6}$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |  |
| $\Psi_{1,1,5}$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |  |
| $\Psi_{1,2,4}$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |  |
| $\Psi_{1,3,3}$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |  |
| $\Psi_{1,4,2}$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |  |
| $\Psi_{1,5,1}$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |  |
| $\Psi_{1,6,0}$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |  |
| $\Psi_{2,0,5}$ | $\checkmark$ | $\checkmark$ | $\checkmark$ | $\checkmark$ |  |
| $\Psi_{2,1,4}$ | $\checkmark$ | $\checkmark$ | $\checkmark$ | $\checkmark$ |  |
| $\Psi_{2,2,3}$ | $\checkmark$ | $\checkmark$ | $\checkmark$ | $\checkmark$ |  |
| $\Psi_{2,3,2}$ | $\checkmark$ | $\checkmark$ | $\checkmark$ | $\checkmark$ |  |
| $\Psi_{2,4,1}$ | $\checkmark$ | $\checkmark$ | $\checkmark$ | $\checkmark$ |  |
| $\Psi_{2,5,0}$ | $\checkmark$ | $\checkmark$ | $\checkmark$ | $\checkmark$ |  |
| $\Psi_{3,0,4}$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |  |
| $\Psi_{3,1,3}$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |  |
| $\Psi_{3,2,2}$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |  |
| $\Psi_{3,3,1}$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |  |
| $\Psi_{3,4,0}$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |  |
| $\Psi_{4,0,3}$ | $\checkmark$ | $\checkmark$ | $\checkmark$ | $\checkmark$ |  |
| $\Psi_{4,1,2}$ | $\checkmark$ | $\checkmark$ | $\checkmark$ | $\checkmark$ |  |
| $\Psi_{4,2,1}$ | $\checkmark$ | $\checkmark$ | $\checkmark$ | $\checkmark$ |  |
| $\Psi_{4,3,0}$ | $\checkmark$ | $\checkmark$ | $\checkmark$ | $\checkmark$ |  |
| $\Psi_{5,0,2}$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |  |
| $\Psi_{5,1,1}$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |  |
| $\Psi_{5,2,0}$ |  | $\checkmark$ | $\checkmark$ | $\checkmark$ |  |
| $\Psi_{6,0,1}$ | $\checkmark$ | $\checkmark$ | $\checkmark$ | $\checkmark$ |  |
| $\Psi_{6,1,0}$ | $\checkmark$ | $\checkmark$ | $\checkmark$ | $\checkmark$ |  |
| $\Psi_{7,0,0}$ |  |  | $\checkmark$ | $\checkmark$ |  |

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