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# A complete basis for a perturbation expansion of the general *N*-body problem

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#### Abstract

We discuss a basis set developed to calculate perturbation coefficients in an expansion of the general N-body problem. This basis has two advantages. First, the basis is complete order-by-order for the perturbation series. Second, the number of independent basis tensors spanning the space for a given order does not scale with N, the number of particles, despite the generality of the problem. At first order, the number of basis tensors is 25 for all N, i.e. the problem scales as  $N^0$ , although one would initially expect an  $N^6$  scaling at first order. The perturbation series is expanded in inverse powers of the spatial dimension. This results in a maximally symmetric configuration at lowest order which has a point group isomorphic with the symmetric group,  $S_N$ . The resulting perturbation series is order-by-order invariant under the N! operations of the  $S_N$  point group which is responsible for the slower than exponential growth of the basis. In this paper, we demonstrate the completeness of the basis and perform the first test of this formalism through first order by comparing to an exactly solvable fully interacting problem of N particles with a two-body harmonic interaction potential.

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## 1. Introduction

In a previous paper [1], we described the development of a perturbation method for the general *S*-wave *N*-body problem through first order. Group theoretic and graphical techniques were used to describe the interacting *N*-body wavefunction for a system of identical bosons with general interactions. Solutions for this problem are known to scale exponentially with *N* requiring that resources be essentially doubled for each particle added [2, 3]. As *N* increases beyond a few tens of particles, this growth makes a direct numerical simulation intractable without approximations given current numerical resources. Typical approximations truncate the Hilbert space of the exact solution by using a basis that spans a smaller Hilbert space or by

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truncating a perturbation series or both [4–20]. With bosonic systems, various Monte Carlo approaches may be employed which scale in a polynomial fashion with N, making larger-N calculations feasible [7–15, 17].

In [1], a perturbation series is developed in inverse powers of the spatial dimension. This results in a maximally symmetric configuration at lowest order having a point group isomorphic to the symmetric group  $S_N$ . The basis used is complete at each order, finite, and, in fact small, having only 25 members at first order, despite the  $N^6$  scaling of the problem at this order.

In this paper, we test this formalism which truncates the perturbation series, but determines each term in the series exactly using group theory and graphical techniques. This perturbation series is order-by-order invariant under the operations of the  $S_N$  point group. The tensor blocks needed at each order can thus be decomposed into a basis also invariant under the  $S_N$  point group. It is this restriction, i.e. the invariance under N! permutations, that stops the growth of the number of basis tensors as N increases, resulting in a basis that is small in contrast to the  $N^6$  growth of the vector space at first order.

We have named the basis tensors, 'binary invariants'. 'Binary' because the elements within a basis tensor are ones or zeros; 'invariants' because the basis tensors are invariant under N! permutations of the particle labels.

This strategy effectively separates the *N* scaling away from the rest of the physics and then tackles the *N*-scaling problem using the symmetry of the  $S_N$  group. The full problem, of course, scales exponentially in *N*, so as higher orders of the perturbation series are included the full exponential *N* scaling of the problem will appear. However, in this methodology, the *N* scaling problem has been compartmentalized away from the rest of the physics and dealt with using group theoretic and graphical techniques; i.e. it becomes a straight mathematical problem. Once this mathematical work, which involves significant analytical effort, has been completed at a given order, it never has to be repeated again for a new interaction or a different number of particles, i.e. the problem now scales as  $N^0$ .

The formalism being tested in this paper has been presented in a series of papers beginning with the isotropic, lowest-order ground-state wavefunction [21], the isotropic, lowest-order ground-state density profile [22] (a brief four page summary of the method at lowest order, along with some lowest-order results, may be found in [23]), and the isotropic, first-order ground-state wavefunction [1].

In section 2, we review the large-dimension point group symmetry and discuss its implications in perturbation theory. In section 3, we discuss the binary invariants themselves and the graphs which label them, and in section 4 we very briefly review the general theory for the wavefunction through first order from [1]. In section 5, we compare the results of the general theory for the wavefunction through first order applied to the problem of the harmonically interacting system under harmonic confinement with an expansion of the exact interacting wavefunction through first order. This work is performed in the appendix where we exactly solve for the wavefunction of the harmonically interacting N-particle problem under harmonic confinement in D dimensions. This exact solution is then expanded through first order in the square root of the inverse dimension of space.

# 2. The large-dimension, point group symmetry and its implications in perturbation theory

As discussed in previous papers, the Hamiltonian and Jacobian-weighted wavefunction and energy are expanded in powers of  $\delta^{1/2}$ , where  $\delta = 1/D$ :

$$\bar{H} = \bar{H}_{\infty} + \delta^{\frac{1}{2}} \bar{H}_{-1} + \delta \sum_{j=0}^{\infty} (\delta^{\frac{1}{2}})^{j} \bar{H}_{j} 
\Phi(\bar{r}_{i}, \gamma_{ij}) = \sum_{j=0}^{\infty} (\delta^{\frac{1}{2}})^{j} \Phi_{j},$$

$$\bar{E} = \bar{E}_{\infty} + \delta^{\frac{1}{2}} \bar{E}_{-1} + \delta \sum_{j=0}^{\infty} (\delta^{\frac{1}{2}})^{j} \bar{E}_{j} ,$$
(1)

where

$$\bar{H}_{\infty} = \bar{E}_{\infty},\tag{2}$$

$$\bar{H}_{-1} = \bar{E}_{2n-1} = 0, \tag{3}$$

$$\bar{H}_{0} = -\frac{1}{2} \frac{}{2} \frac{}{2} G_{\nu_{1},\nu_{2}} \partial_{\bar{y}_{\nu_{1}}} \partial_{\bar{y}_{\nu_{2}}} + \frac{1}{2} \frac{}{2} \frac{}{2} F_{\nu_{1},\nu_{2}} \bar{y}_{\nu_{1}}' \bar{y}_{\nu_{2}}' + \frac{}{0} \frac{}{0} F, \qquad (4)$$

$$\bar{H}_{1} = -\frac{1}{2} \frac{{}^{(1)}}{{}^{3}} G_{\nu_{1},\nu_{2},\nu_{3}} \bar{y}_{\nu_{1}}' \partial_{\bar{y}_{\nu_{2}}} \partial_{\bar{y}_{\nu_{3}}'} - \frac{1}{2} \frac{{}^{(1)}}{{}^{1}} G_{\nu} \partial_{\bar{y}_{\nu}'} + \frac{1}{3!} \frac{{}^{(1)}}{{}^{3}} F_{\nu_{1},\nu_{2},\nu_{3}} \bar{y}_{\nu_{1}}' \bar{y}_{\nu_{2}}' \bar{y}_{\nu_{3}}' + \frac{{}^{(1)}}{{}^{1}} F_{\nu} \bar{y}_{\nu}'.$$
(5)

The internal displacement coordinate vector  $\bar{y}'_{\nu}$  is a column vector composed of the displacement radii  $\bar{r}'_i$  and the displacement angle cosines  $\bar{y}'_{i,j}$ :

$$\bar{\boldsymbol{y}}' = \left(\frac{\bar{r}'}{\bar{\gamma}'}\right), \quad \text{where} \quad \left(\begin{array}{c} \frac{\overline{\gamma}'_{12}}{\overline{\gamma}'_{13}}\\ \frac{\overline{\gamma}'_{23}}{\overline{\gamma}'_{14}}\\ \frac{\overline{\gamma}'_{24}}{\overline{\gamma}'_{24}}\\ \frac{\overline{\gamma}'_{34}}{\overline{\gamma}'_{15}}\\ \frac{\overline{\gamma}'_{15}}{\overline{\gamma}'_{25}}\\ \vdots\\ \frac{\overline{\gamma}'_{N-2,N}}{\overline{\gamma}'_{N-1,N}}\end{array}\right), \quad (6)$$

and is related to the dimensionally scaled internal coordinates by

$$\bar{r}_i = \bar{r}_\infty + \delta^{1/2} \bar{r}'_i$$
 and  $\gamma_{ij} = \gamma_\infty + \delta^{1/2} \overline{\gamma}'_{ij}$ , (7)

where  $\bar{r}_i$  are the dimensionally scaled radii and  $\gamma_{ij}$  are the angle cosines between the position vectors of the *N* particles.

The superprescript on the F and G tensors in parentheses in equations (3)–(5) denotes the order in  $\delta^{1/2}$  that the term enters (harmonic being zeroth order). The subprescripts denote the rank of the tensors.

In general,  $\bar{H}_n$  is of order n + 2 in the elements and derivatives of  $\bar{y}'$  (second order in the derivatives), and formed of either all even or all odd powers of the elements and derivatives of  $\bar{y}'$  when *n* is even or odd, respectively.

According to equation (7) the system localizes as  $D \to \infty$  on a configuration centered about  $\bar{r}_i = \bar{r}_{\infty}$  and  $\gamma_{ij} = \gamma_{\infty}$ . This structure has the highest degree of symmetry where all particles are equidistant from the center of the trap and equiangular from each other (a configuration that is only possible in higher dimensions). The point group of this structure is isomorphic to  $S_N$  which in effect interchanges the particles in the large dimension structure. This together with the fact that the full *D*-dimensional Hamiltonian,  $\hat{H}$ , is invariant under particle exchange means the expansion of equation (1) is order-by-order invariant under this  $S_N$  point group, i.e.  $\bar{H}_j$  are each invariant under the  $S_N$  point group. This greatly restricts the F and G tensors of equations (4) and (5). In three dimensions a corresponding *N*-particle structure would have a point group of lower symmetry, i.e. one not isomorphic to  $S_N$  despite the fact that all of the particles are identical. It is this profound restriction on the F and G tensors from the  $S_N$  point group symmetry, which in itself is a direct consequence of developing a perturbation theory about the large-dimension limit, that allows for an essentially analytic solution of the problem at a given order in the perturbation theory for *any N*. For example, with a third-rank tensor, instead of  $(N(N + 1)/2)^3$  possible independent elements (a number which becomes quickly intractable since, for example, with only ten particles this would be more than a million elements), the  $S_N$  point group symmetry restricts the number of independent elements to only 23, independent of the value of N.

#### 2.1. The reducibility of the **F** and **G** tensors under $S_N$

The maximally symmetric point group  $S_N$ , together with the invariance of the full Hamiltonian under particle interchange, requires that the *F* and *G* tensors be invariant under the interchange of particle labels (the  $S_N$  group). In fact the various blocks of the *F* and *G* tensors are themselves invariant under particle interchange induced by the point group. For example,  ${}^{(1)}_{3}F^{rr\gamma}_{i,j,(kl)}$  is never transformed into  ${}^{(1)}_{3}F^{\gamma\gamma\gamma}_{(ij),(kl)(mn)}$ , i.e. the *r* and  $\gamma$  labels are preserved since the  $S_N$  group does not transform an  $\bar{r}'_i$  coordinate into a  $\overline{\gamma}'_{(ij)}$  coordinate.

the  $S_N$  group does not transform an  $\bar{r}'_i$  coordinate into a  $\bar{\gamma}'_{(ij)}$  coordinate. The various  $r - \gamma$  blocks of the *F* and *G* tensors may be decomposed into invariant, and, this time irreducible, blocks. Thus for example,  ${}^{(0)}_2 Q$  may be decomposed into the blocks

$$\begin{array}{ll} \overset{(0)}{2} Q_{i,i}^{rr} & \forall i \\ \overset{(0)}{2} Q_{i,j}^{rr} & \forall i \neq j \\ \overset{(0)}{2} Q_{i,(j)}^{r\gamma} & \forall i \neq j \\ \overset{(0)}{2} Q_{i,(k)}^{r\gamma} & \forall i \neq j < k \\ \overset{(0)}{2} Q_{i,(jk)}^{r\gamma} & \forall i \neq j < k \\ \overset{(0)}{2} Q_{(ij),(ij)}^{\gamma\gamma} & \forall i < j \\ \overset{(0)}{2} Q_{(ij),(ik)}^{\gamma\gamma} & \forall i < j \neq k > i \\ \overset{(0)}{2} Q_{(ij),(k)}^{\gamma\gamma} & \forall i \neq j \neq k \neq l, \\ i < j, \quad k < l \end{array}$$

$$\begin{array}{l} (8) \\ \end{array}$$

all of which remain disjoint from one another under the  $S_N$  group. Significantly, invariance under particle interchange requires that tensor elements related by a label permutation induced by the point group must be equal. This requirement partitions the set of tensor elements for each block into disjoint subsets of identical elements. Consider the elements of the  $\binom{00}{2}Q_{i,i}^{rr}$  block. The element  $\binom{00}{2}Q_{1,1}^{rr}$  belongs to a set of *N* elements (of the form  $\binom{00}{2}Q_{i,i}^{rr}$ ) which are related by a permutation induced by the point group, and therefore must have equal values. Likewise, the element  $\binom{00}{2}Q_{1,2}^{rr}$  belongs to a set of N(N-1) elements related by a permutation induced by the point group and sharing a common value. Proceeding in this fashion, we observe that the blocks of the lowest-order tensors are partitioned into the following set of identical elements which remain disjoint under particle interchange:

$${}^{(0)}_{2}Q^{rr}_{i,i} = {}^{(0)}_{2}Q^{rr}_{k,k} \quad \forall i \quad \text{and} \quad k,$$
(9)

$${}^{(0)}_{2} Q^{rr}_{i,j} = {}^{(0)}_{2} Q^{rr}_{k,l} \quad \forall i \neq j \quad \text{and} \quad k \neq l,$$
(10)

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$${}^{(0)}_{2}\mathcal{Q}^{r\gamma}_{i,(ik)} = {}^{(0)}_{2}\mathcal{Q}^{r\gamma}_{l,(lm)} = {}^{(0)}_{2}\mathcal{Q}^{r\gamma}_{n,(pn)} \quad \forall i < k, \qquad l < m \quad \text{and} \quad n > p,$$
(11)

$${}^{(0)}_{2} Q^{r\gamma}_{i,(jk)} = {}^{(0)}_{2} Q^{r\gamma}_{l,(mn)} \quad \forall i \neq j < k \quad \text{and} \quad l \neq m < n,$$
(12)

$${}^{(0)}_{2} Q^{\gamma \gamma}_{(ii)(ij)} = {}^{(0)}_{2} Q^{\gamma \gamma}_{(kl)(kl)} \quad \forall i < j \quad \text{and} \quad k < l$$
(13)

$${}^{(0)}_{2} Q^{\gamma \gamma}_{(ij),(ik)} = {}^{(0)}_{2} Q^{\gamma \gamma}_{(lm),(ln)} \quad \forall i < j \neq k > i \quad \text{and} \quad l < m \neq n > l,$$
(14)

$${}^{(0)}_{2} Q^{\gamma\gamma}_{(ij),(kl)} = {}^{(0)}_{2} Q^{\gamma\gamma}_{(mn),(pq)} \quad \forall i \neq j \neq k \neq l \quad \text{and} \quad m \neq n \neq p \neq q$$

$$i < i, \quad k < l \qquad m < n, \quad p < q.$$

$$(15)$$

The lowest-order block matrices contain the sets of elements in equations (9)–(15) arranged in an intricate pattern. A similar, but more involved partitioning occurs for higher rank F and G tensors.

In [1] it was shown that this decomposition could be expressed in terms of binary tensors which are invariant under  $S_N$  and are labeled by graphs. We term these binary tensors, binary invariants.

#### 3. Binary invariants

3.1. Introducing graphs

**Definition 1.** A graph  $\mathcal{G} = (V, E)$  is a set of vertices V and edges E. Each edge has one or two associated vertices, which are called its endpoints [24].

For example,  $\bigcirc$  is a graph  $\mathcal{G}$  with three vertices and three edges. We allow our graphs to include loops and multiple edges<sup>3</sup>. A graph contains information regarding the connectivity of edges and vertices only: the orientation of edges and vertices has no consequence.

We introduce a mapping which associates each tensor element with a graph as follows:

- (i) draw a labeled vertex  $(\cdot i)$  for each distinct index in the set of indices of the element;
- (ii) draw an edge  $(\stackrel{i}{\bullet} \stackrel{j}{\bullet})$  for each double index (ij);
- (iii) draw a 'loop' edge  $(\bigcirc i)$  for each distinct single index *i*.

*i* For example, the graph corresponding to the tensor element  ${}^{(0)}_2 Q^{r\gamma}_{i,(ij)}$  under this mapping is  $\bigcirc j$ .

Two graphs with the same number of vertices and edges that are connected in the same way are called *isomorphic*. The elements of the  $S_N$  group are permutation operations which interchange particle labels. Two elements with graphs that are not isomorphic are never related by a permutation of the  $S_N$  group. We label each set of isomorphic graphs by a graph with no vertex labels. Denoting the set of unlabeled graphs for each block as  $\mathbb{G}_{X_1,X_2,...,X_n}$ , where *n* is the rank of the tensor block (and therefore the number of edges in each graph in the set) and *X* is *r* or  $\gamma$ , we have

$$\begin{aligned}
 \mathbb{G}_{rr} &= \{ \bigcirc, \bigcirc, \bigcirc \bigcirc \} \\
 \mathbb{G}_{\gamma r} &= \{ \bigcirc, \bigcirc, \frown, \frown \leftrightarrow \} \\
 \mathbb{G}_{\gamma \gamma} &= \{ \bigcirc, \_, \_, \fbox \}
 \end{aligned}$$
(16)

<sup>3</sup> Strictly speaking, this is a 'loop multigraph'. The definition of a graph does not allow for multiple edges between a pair of vertices nor a 'loop' edge with common endpoints.

Now consider a tensor, for which all of the elements labeled by a single isomorphic set of graphs are equal to unity, while all of the other elements labeled by graphs heteromorphic to this single set of isomorphic graphs are equal to zero. We term this tensor a binary invariant,  $[B(\mathcal{G})]_{\nu_1,\nu_2,...}$  since it is invariant under the  $S_N$  group, and we label it by the graph  $\mathcal{G}$ , without particle labels at the vertices, for the non-zero elements all of which are equal to unity. Thus each of the above graphs denotes a binary invariant,  $[B(\mathcal{G})]_{\nu_1,\nu_2,...}$ . Explicit expressions for these binary invariants for arbitrary N may be found in the EPAPS document [25].

#### 3.2. Binary invariants are a basis

That the small number of binary invariants are a complete basis with which to represent any  $S_N$  invariant tensor in the N(N + 1)/2-dimensional  $\bar{r}' - \bar{\gamma}'$  space can be seen as follows.

**Lemma 1.** The set of binary invariants,  $[B(\mathcal{G})]_{\nu_1,\nu_2,\dots}$ , for all  $\mathcal{G} \in \mathbb{G}$  are linearly independent.

**Proof.** This follows from the fact that no binary invariant shares a non-zero element with another binary invariant for a different graph.  $\Box$ 

**Lemma 2.** The set of binary invariants for all  $\mathcal{G} \in \mathbb{G}$  spans the invariant tensor space.

**Proof.** From the mapping of section 3.1 above, relating graphs to tensor elements in the  $\bar{r}' - \bar{\gamma}'$  space, every tensor element is related to an unlabeled graph, and so the binary invariants for all possible unlabeled graphs span the invariant tensor subspace.

**Theorem 1.** The set of binary invariants  $\{B(\mathcal{G}) : \mathcal{G} \in \mathbb{G}\}$  forms a basis for the  $S_N$  variant Hamiltonian coefficient tensors.

**Proof.** This result follows from the definition of a basis and that the set of binary invariants for all  $\mathcal{G} \in \mathbb{G}$  is linearly independent and spans the vector space.

As shown in [26] this result generalizes to any group with any set of tensors invariant under that group.

Therefore, we may resolve the Q tensors at any order as a finite linear combination of binary invariants:

$${}^{(O)}_{R} \mathcal{Q}^{\text{block}}_{\nu_{1},\nu_{2},\dots,\nu_{R}} = \sum_{\mathcal{G} \in \mathbb{G}_{\text{block}}} \mathcal{Q}^{\text{block}}(\mathcal{G})[B^{\text{block}}(\mathcal{G})]_{\nu_{1},\nu_{2},\dots,\nu_{R}},$$
(18)

where  $\mathbb{G}_{block}$  represents the set of graphs present in the order-O, rank-R tensor block  ${}^{(O)}_{R}Q^{block}$ , and the binary invariant  $B^{block}(\mathcal{G})$  has the same dimensions as the original Q tensor block. The scalar quantity  $Q^{block}(\mathcal{G})$  is the expansion coefficient.

The resolution of symmetric tensor blocks in the basis of binary invariants in equation (18) represents a generalization of a technique used at lowest order in [21, 27] to arbitrary order. This equation also separates the specific interaction dynamics present in  $Q^{\text{block}}(\mathcal{G})$  from the point group symmetry embodied in  $B^{\text{block}}(\mathcal{G})$ .

#### 4. The wavefunction through first order

#### 4.1. Lowest-order ground-state wavefunction

Since the Hamiltonian of the lowest-order wavefunction (equation (4)) has the form of a N(N + 1)/2-dimensional coupled harmonic oscillator, the lowest-order wavefunction will be a product of one-dimensional, harmonic-oscillator, normal-mode functions.

The lowest-order wavefunction,  ${}_{g}\Phi_{0}(\mathbf{q}')$ , for the ground state is given by

$${}_{g}\Phi_{0}(\mathbf{q}') = \prod_{\nu=1}^{P} \phi_{0}(\sqrt{\bar{\omega}_{\nu}}q_{\nu}'), \qquad (19)$$

where

$$\phi_0(\sqrt{\bar{\omega}_\nu}q'_\nu) = \left(\frac{\bar{\omega}_\nu}{\pi}\right)^{\frac{1}{4}} \exp\left(-\frac{1}{2}\bar{\omega}_\nu {q'_\nu}^2\right).$$
(20)

There are N(N+1)/2 normal modes and up to N(N+1)/2 distinct frequencies, a number which would become impossibly large to solve for if it were not for the  $S_N$  point group symmetry expressed in the invariance of the F and G tensors, and the small, N-independent number of binary invariants spanning the invariant tensor spaces. In [21, 27, 28] we have used this  $S_N$ point group symmetry to derive both the frequencies and normal modes of the lowest-order, Jacobian-weighted wavefunction for arbitrary N. This analysis results in only five distinct frequencies, associated with center-of-mass and breathing modes, radial and angular singly excited state modes, and phonon modes. Each of these frequencies is associated with a set of normal modes which transforms under an irreducible representation of the  $S_N$  point group.

#### 4.2. First-order wavefunction

Using the  $S_N$  point group symmetry expressed in the invariance of the F and G tensors, and the small, *N*-independent number of binary invariants spanning the invariant tensor spaces, in [1] we have also derived the first-order correction to the lowest-order, harmonic wavefunction. If we write

$$\Phi(\mathbf{q}') = \left(1 + \delta^{\frac{1}{2}}\hat{\Delta}\right)\Phi_0(\mathbf{q}') + O(\delta),\tag{21}$$

then  $\hat{\Delta}$  satisfies the commutator equation

$$[\hat{\Delta}, \hat{H}_0]\Phi_0 = \hat{H}_1\Phi_0. \tag{22}$$

To solve this equation, we note that since  $\Phi_0(\mathbf{q}')$  is a Gaussian function, the derivatives in  $\hat{H}_1$ and  $\hat{H}_0$  written in normal coordinates 'bring down' normal coordinates from the exponent so that  $\hat{H}_1$  effectively becomes a third-order polynomial of only odd powers in  $\mathbf{q}'$ . Then from equation (22)  $\hat{\Delta}$  is a cubic polynomial and of only odd powers in the normal modes. When  $\hat{\Delta}$  is re-expressed in terms of internal displacement coordinates,  $\mathbf{r}'$  and  $\gamma'$ , it is cubic and of only odd powers in these internal displacement coordinates.

The ground-state wavefunction is also scalar under  $S_N$ , and so when it is expressed in terms of internal displacement coordinates it involves binary invariants which take powers of the internal displacement coordinates and couple them together to produce a scalar under  $S_N$ .

# 5. A test of the theory: the harmonically confined, harmonically interacting system

The general theory developed in [1, 21], and briefly reviewed in this paper, is extensive, and we test it on a non-trivial, interacting, analytic solvable model: the harmonically- interacting system of N particles under harmonic confinement:

$$H = \frac{1}{2} \left( \sum_{i}^{N} \left[ -\frac{\partial^2}{\partial r_i^2} + \omega_t^2 r_i^2 \right] + \sum_{i < j}^{N} \omega_p^2 r_{ij}^2 \right).$$
(23)

# 5.1. The wavefunction through first order

In the appendix, we independently solve the harmonically confined, harmonically interacting system of N particles exactly for the ground-state wavefunction (see equation (A.6)), and then from this derive the exact perturbation series for the N-body wavefunction (weighted by a Jacobian) through first order:

$$\Psi_J = \left(\frac{1}{\sqrt[4]{\pi}}\right)^{\frac{N(N+1)}{2}} \left(1 + \frac{1}{2}\delta^{\frac{1}{2}}\Delta_{\bar{\mathbf{y}}'} + O(\delta)\right) \exp\left(-[\bar{\mathbf{y}}']^T \bar{\Omega}_{\bar{\mathbf{y}}'} \bar{\mathbf{y}}'\right).$$
(24)

where

$$\Delta_{\bar{\mathbf{y}}'} = \Delta(\mathbb{Q})[B(\mathbb{Q})]_{i}\bar{r}'_{i} + \Delta(\mathbb{Q})[B(\mathbb{Q})]_{(ij)}\bar{\gamma}'_{(ij)} + \Delta(\mathbb{Q})[B(\mathbb{Q})]_{i,j,k}\bar{r}'_{i}\bar{r}'_{j}\bar{r}'_{k}$$

$$+\Delta(\mathbb{Q})[B(\mathbb{Q})]_{(ij),k,l}\bar{\gamma}'_{(ij)}\bar{r}'_{k}\bar{r}'_{l} + (\Delta(\mathbb{Q})[B(\mathbb{Q})]_{(ij),(kl),(mn)}$$

$$+\Delta(\mathbb{Q})[B(\mathbb{Q})]_{(ij),(kl),(mn)} + \Delta(\mathbb{Q})[B(\mathbb{Q})]_{(ij),(kl),(mn)}$$

$$+\Delta(\mathbb{Q})[B(\mathbb{Q})]_{(ij),(kl),(mn)} + \Delta(\mathbb{Q})[B(\mathbb{Q})]_{(ij),(kl),(mn)}$$

$$+\Delta(\mathbb{Q})[B(\mathbb{Q})]_{(ij),(kl),(mn)} + \Delta(\mathbb{Q})[B(\mathbb{Q})]_{(ij),(kl),(mn)}$$

$$+\Delta(\mathbb{Q})[B(\mathbb{Q})]_{(ij),(kl),(mn)})\bar{\gamma}'_{(ij)}\bar{\gamma}'_{(kl)}\bar{\gamma}'_{(mn)}, \qquad (25)$$

$$\begin{split} [\bar{\mathbf{y}}']^T \bar{\Omega}_{\bar{\mathbf{y}}'} \bar{\mathbf{y}}' &= (\Delta(\bigcirc) [B(\bigcirc)]_{i,j} + \Delta(\bigcirc \bigcirc) [B(\bigcirc \bigcirc)]_{i,j}) \bar{r}'_i \bar{r}'_j \\ &+ \Delta(\bigcirc) [B(\bigcirc)]_{(ij),k} \bar{\gamma}'_{(ij)} \bar{r}'_k + (\Delta(\bigcirc) [B(\bigcirc)]_{(ij),(kl)} \\ &+ \Delta(\_) [B(\_])]_{(ij),(kl)} + \Delta(\bigcirc) [B(\bigcirc]]_{(ij),(kl)}) \bar{\gamma}'_{(ij)} \bar{\gamma}'_{(kl)}. \end{split}$$
(26)

Repeated indices  $i, j, \ldots$  imply summation from 1 to N, while repeated index pairs (ij), etc imply the ordered sum  $1 \leq i \leq j \leq N$ . For example,  $[B(\frown)]_{i,j,k}\bar{r}'_i\bar{r}'_j\bar{r}'_k = \bar{r}'_1{}^3 + \bar{r}'_2{}^3 + \cdots + \bar{r}'_N{}^3$ . In the above expressions for  $\Delta_{\bar{\mathbf{y}}'}$  and  $[\bar{\mathbf{y}}']^T \bar{\Omega}_{\bar{\mathbf{y}}'}\bar{\mathbf{y}}'$ , we are building up the invariant polynomials in  $\bar{r}'_i$  and  $\bar{\gamma}'_{(kl)}$  using the binary invariants as our building blocks. The scalar coefficients,  $\Delta(\mathcal{G})$  are (derived in the appendix)

$$\Delta(\mathbb{Q}) = -\frac{1}{\bar{r}_{\infty}},\tag{27}$$

$$\Delta( \to) = \mathcal{A} \, 6 \, (N+1) \gamma_{\infty}, \tag{28}$$

$$\Delta(\bigcirc) = \frac{1}{3\bar{r}_{\infty}^3},\tag{29}$$

$$\Delta(\bigcirc \frown) = \frac{\lambda - 1}{N},\tag{30}$$

$$\Delta(\bigcirc) = \mathcal{A}(\mathcal{B} + \mathcal{CD}),\tag{31}$$

$$\Delta(\varDelta) = \mathcal{A}(\mathcal{B} + \mathcal{C}\mathcal{E} + \mathcal{F}), \tag{32}$$

$$\Delta(\bigcirc \rightarrow) = \mathcal{A}\left(\mathcal{B} + \mathcal{C}\left(\frac{\mathcal{D}}{3} + \frac{2\mathcal{E}}{3}\right)\right), \tag{33}$$
$$\Delta(\uparrow) = \mathcal{A}(\mathcal{B} + \mathcal{C}\mathcal{E}), \tag{34}$$

$$\Delta(---) = \mathcal{A}(\mathcal{B} + \mathcal{C}\mathcal{E}), \tag{34}$$

$$\Delta(\underline{\square}) = \mathcal{A}\left(\mathcal{B} + \frac{2\mathcal{C}\mathcal{E}}{3} - \mathcal{G}\right),\tag{35}$$

$$\Delta(\bigcirc) = \mathcal{A}\left(\mathcal{B} + \frac{\mathcal{C}\mathcal{D}}{3} + 2\mathcal{G}\right),\tag{36}$$

$$\Delta(\square) = \mathcal{A}\left(\mathcal{B} + \frac{cc}{3}\right),\tag{37}$$

$$\Delta(\Xi) = \mathcal{AB}, \tag{38}$$

$$\Delta(\bigcirc) = \lambda_{\text{eff}} + \frac{\lambda - 1}{2N} (\lambda_{\text{eff}} - 1), \tag{39}$$
$$\Delta(\bigcirc \bigcirc) = \frac{\gamma_{\infty}}{2}, \tag{40}$$

$$\Delta(\bigcirc \bigcirc) = \frac{1}{2}, \tag{40}$$
$$\Delta(\bigcirc \rightarrow) = \bar{r}_{\infty}, \tag{41}$$

$$\Delta(\bigcirc \rightarrow) = r_{\infty}, \tag{41}$$

$$\Delta(\{\cdot\}) = \mathcal{H}(I+\mathcal{I}), \tag{42}$$

$$\Delta(\underline{I}) = \mathcal{H}\left(\mathcal{I} - \frac{r_{\infty}}{2}\right),\tag{43}$$

In the above equations, we have defined

$$\lambda = \sqrt{1 + N\lambda_p^2},\tag{45}$$

$$\lambda_p = \frac{\omega_p}{\omega_t},\tag{46}$$

$$\gamma_{\infty} = \frac{(\lambda - 1)}{(N + (\lambda - 1))},\tag{47}$$

$$\bar{r}_{\infty}^{2} = \frac{1}{2(1 + (N - 1)\gamma_{\infty})} = \frac{N + (\lambda - 1)}{2\lambda N},$$
(48)

$$\lambda_{\text{eff}} = \frac{N\lambda}{N+\lambda-1},\tag{49}$$

$$\mathcal{A} = \frac{1}{6(1 - \gamma_{\infty})(1 + (N - 1)\gamma_{\infty})},$$
(50)

$$\mathcal{B} = -\frac{8\gamma_{\infty}^{3}}{(1 - \gamma_{\infty})^{2}(1 + (N - 1)\gamma_{\infty})^{2}},$$
(51)

$$C = -\frac{6\gamma_{\infty}}{(1 - \gamma_{\infty})^2 (1 + (N - 1)\gamma_{\infty})},$$
(52)  

$$D = (1 + (N - 3)\gamma_{\infty})$$
(53)

$$\mathcal{D} = (1 + (N - 3)\gamma_{\infty}), \tag{53}$$

$$\mathcal{E} = -\gamma_{\infty},\tag{54}$$

**Table 1.** Fractional difference,  $\Delta \Delta(\mathcal{G}) = (\Delta_{ind}(\mathcal{G}) - \Delta_{gen}(\mathcal{G}))/\Delta_{ind}(\mathcal{G})$ , between the independently derived (ind) and the general formalism (gen) rank-3, rank-2, and rank-1 binary invariant coefficients when  $N = 10\,000$  and  $\lambda = 10$ .

| G           | $\Delta \left[ \bigtriangleup(\mathcal{G}) \right]$ | ${\mathcal G}$ | $\Delta\left[\bigtriangleup(\mathcal{G})\right]$ | ${\cal G}$          | $\Delta\left[ \bigtriangleup(\mathcal{G})\right]$ |
|-------------|---|----------------|--|---------------------|---|
| $\odot$     | $7.0 	imes 10^{-16}$                                | Ц              | $-1.5\times10^{-16}$                             | 00                  | $-3.6 \times 10^{-16}$                            |
| 0-0         | $2.3 	imes 10^{-11}$                                | $\bigcirc$     | $-6.0 \times 10^{-13}$                           | $\bigcirc \bigcirc$ | $-5.1\times10^{-11}$                              |
| $\ominus$   | $-4.1 \times 10^{-16}$                              | $\Box$         | $3.7 \times 10^{-16}$                            | $\bigcirc$          | $9.6 	imes 10^{-15}$                              |
| $\varDelta$ | $-1.3 \times 10^{-16}$                              | Ξ              | $-2.1 \times 10^{-13}$                           | 0                   | $-3.7 \times 10^{-16}$                            |
| $\frown$    | $-6.1 	imes 10^{-16}$                               | $\bigcirc$     | $-8.4 \times 10^{-7}$                            |                     | $-2.2\times10^{-16}$                              |
|             | $1.2 	imes 10^{-16}$                                | -              | $8.4 	imes 10^{-10}$                             |                     | $2.5 	imes 10^{-14}$                              |

$$\mathcal{F} = \frac{(1+(N-4)\gamma_{\infty})}{(1-\gamma_{\infty})^2},\tag{55}$$

$$\mathcal{G} = \frac{\gamma_{\infty}}{(1 - \gamma_{\infty})^2},\tag{56}$$

$$\mathcal{H} = \frac{1}{2(1 - \gamma_{\infty})^2 (1 + (N - 1)\gamma_{\infty})},$$
(57)

$$\mathcal{I} = \frac{\gamma_{\infty}^2}{(1 + (N - 1)\gamma_{\infty})},\tag{58}$$

$$\mathcal{J} = \frac{1 + (N-3)\gamma_{\infty}}{2}.$$
(59)

This solution through first order is then compared with the wavefunction derived from the general formalism of [1] (see equations (33) and (117)) and implemented in Mathematica [29] code. For the case of the general formalism, from equations (19) and (20) we find that

$$\bar{\Omega}_{\bar{\mathbf{y}}'} = \mathbf{V}^T \bar{\Omega}_{\mathbf{q}'} \mathbf{V},\tag{60}$$

$$[\bar{\Omega}_{q'}]_{\nu_1,\nu_2} = \delta_{\nu_1,\nu_2}\bar{\omega}_{\nu_1},\tag{61}$$

and V is the matrix transforming from the internal displacement coordinate vector  $\bar{\mathbf{y}}'$  to the normal mode coordinate vector  $\mathbf{q}'$ . The polynomial  $\Delta$  of equation (21) is similarly transformed from a normal coordinate basis to  $\Delta_{\bar{\mathbf{y}}'}$  of equation (24) in the internal coordinate basis.

In tables 1–4 we compare the binary invariant coefficients,  $\Delta(\mathcal{G})$ , from the general theory of [1, 21] with the above results derived from the full exact, independent solution above for N = 10000 particles and two different interparticle interaction strengths,  $\lambda$ . One value of  $\lambda$  features strongly attractive harmonic interparticle interactions, while the other is for a weakly bound system with repulsive interparticle interactions (negative  $\lambda$ ) for  $\lambda$  just above the dissociation threshold at  $\lambda = -1/\sqrt{N}$ .

In both cases, to within round-off-error determined by the machine precision, exact agreement is found, confirming the correctness of the general formalism of [1], and its implementation in Mathematica [29] coding.

**Table 2.** Rank-3 and rank-2 binary invariant coefficient,  $\triangle_{\text{gen}}(\mathcal{G})$ , from the general *Mathematica* code when  $N = 10\,000$  and  $\lambda = 10$ . All of these coefficients are exactly zero in the exactly soluble independent solution.

| G                   | $	riangle(\mathcal{G})$ | ${\cal G}$              | $\triangle(\mathcal{G})$ |
|---------------------|-------------------------|-------------------------|--------------------------|
| 80                  | $2.3 	imes 10^{-11}$    | 00                      | $-2.9 \times 10^{-15}$   |
| ŏ00                 | $1.1 	imes 10^{-11}$    | $\circ \circ$           | $7.8 	imes 10^{-19}$     |
| 8.                  | $2.4 	imes 10^{-15}$    | <u> </u>                | $4.1 \times 10^{-19}$    |
| $\tilde{\circ}$     | $2.2 \times 10^{-15}$   | Lo                      | $9.8 	imes 10^{-17}$     |
| $\underline{\circ}$ | $2.0 	imes 10^{-15}$    | LО                      | $1.0 \times 10^{-19}$    |
| $\bigcirc \bigcirc$ | $8.2 \times 10^{-16}$   | $\underline{-}^{\circ}$ | $6.2 \times 10^{-20}$    |
| $\bigcirc$ $-$      | $-1.2\times10^{-17}$    | $\Box \circ$            | $2.1 \times 10^{-20}$    |

**Table 3.** Fractional difference,  $\Delta \Delta(\mathcal{G}) = (\Delta_{ind}(\mathcal{G}) - \Delta_{gen}(\mathcal{G}))/\Delta_{ind}(\mathcal{G})$ , between the independently derived (ind) and general formalism (gen) rank-3, rank-2 and rank-1 binary invariant coefficients when  $N = 10\,000$  and  $\lambda^2 = -1/10\,000 + 10^{-10}$ .

| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$   |                         |   |                |   |                     |   |
|---|-------------------------|---|----------------|---|---------------------|---|
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$   | G                       | $\Delta \left[ \bigtriangleup(\mathcal{G}) \right]$ | ${\mathcal G}$ | $\Delta \left[ \bigtriangleup(\mathcal{G}) \right]$ | ${\cal G}$          | $\Delta \left[ \bigtriangleup(\mathcal{G}) \right]$ |
| $\begin{array}{c ccccccccccccccccccccccccccccccccccc$   | $\overline{\mathbb{Q}}$ | $1.6 	imes 10^{-11}$                                | Ц              | $-2.0 \times 10^{-8}$                               | $\bigcirc$          | $-2.6 \times 10^{-11}$                              |
| $ \begin{array}{cccccccccccccccccccccccccccccccccccc$   | $\sim$                  | $-3.8 	imes 10^{-8}$                                | $\odot$        | $1.7 \times 10^{-13}$                               | $\bigcirc \bigcirc$ | $-1.1\times10^{-9}$                                 |
| $ \begin{array}{c ccccccccccccccccccccccccccccccccccc$  | $\ominus$               | $2.5 	imes 10^{-8}$                                 | $\Box$         | $2.1 \times 10^{-11}$                               | $\bigcirc$          | $6.8 	imes 10^{-13}$                                |
| $\bigcirc - 2.5 \times 10^{-8} \bigcirc 1.7 \times 10^{-3} \ \ 1.6 \times 10^{-3} \ \ 2.2 \times 10^{-5} \ \ - 1.7 \times 10^{-10} \ \ - 3.8 \times 10^{-3} \ \ - 3.8 \times 1$ | Δ                       | $-3.8 	imes 10^{-8}$                                | Ξ              | $-3.0\times10^{-14}$                                | $\bigcirc$          | $-1.6\times10^{-7}$                                 |
|   | $\bigcirc \neg$         | $2.5 	imes 10^{-8}$                                 | Q              | $1.7 \times 10^{-3}$                                |                     | $1.6 	imes 10^{-10}$                                |
|   | <u> </u>                | $2.2 	imes 10^{-5}$                                 | -              | $-1.7\times10^{-10}$                                |                     | $-3.8 \times 10^{-13}$                              |

**Table 4.** Rank-3 and rank-2 binary invariant coefficient,  $\triangle_{\text{gen}}(\mathcal{G})$ , from the general *Mathematica* code when  $N = 10\,000$  and  $\lambda^2 = -1/10\,000 + 10^{-10}$ . All of these coefficients are exactly zero in the exactly soluble independent solution.

| G                    | $\triangle(\mathcal{G})$ | ${\mathcal G}$             | $\triangle(\mathcal{G})$ |
|----------------------|--------------------------|----------------------------|--------------------------|
| 80                   | $-4.8 \times 10^{-20}$   | 00                         | $2.8 \times 10^{-10}$    |
| ŎQQ                  | $7.9\times10^{-24}$      | $\circ \circ$              | $-1.7\times10^{-14}$     |
| 8.                   | $1.9\times10^{-12}$      | .Ç.                        | $-2.8 	imes 10^{-14}$    |
| $\tilde{\mathbf{O}}$ | $-1.9\times10^{-16}$     | Lo                         | $5.3 	imes 10^{-14}$     |
| $\underbrace{00}$    | $-2.6\times10^{-19}$     | LО                         | $-1.2\times10^{-17}$     |
| $\circ \circ$        | $3.8 \times 10^{-20}$    | $\underline{-}^{\bigcirc}$ | $-5.0 	imes 10^{-18}$    |
| $\circ$ –            | $8.1\times10^{-20}$      | $\Box \circ$               | $3.3 	imes 10^{-20}$     |
|                      |                          |                            |                          |

## 6. Summary and conclusions

In this paper we performed the first test of a general formalism from [1] for a fully interacting *N*-body wavefunction through first order in a perturbation expansion. This formalism was verified by comparison to a fully interacting, exactly solvable model problem.

The resources required for a solution to a general *N*-body problem are understood to scale at least exponentially with N, making it very challenging to solve for large-N systems [2, 3]. The present perturbation series will scale exponentially in N if summed to all orders.

However at first order, the number of terms scale as  $N^6$ , a scaling, while greatly improved, still remains challenging. Nonetheless, this  $N^6$  scaling is tamed by expanding the perturbation series about a point where the *N*-body system has a highly symmetric structure. In the process, the *N*-scaling aspect also effectively separates away from the rest of the physics allowing the *N* scaling to be treated as a straight mathematical issue, which upon solution yields an  $N^0$  scaling.

This highly symmetric structure for arbitrary N is obtained as the number of spatial dimensions approaches infinity, resulting in a configuration whose point group is isomorphic to the  $S_N$  group. All terms in the perturbation series for the Hamiltonian are then invariant under the N! elements of the  $S_N$  group, allowing an expansion in a basis that is also invariant under these N! operations. This restriction results in a comparatively small basis at each order which is independent of N. There are only seven binary invariants at lowest order for any value of N, and 25 at next order independent of N (except when N is quite small when the number is even lower). In this paper we demonstrated the completeness of this basis at all orders. Thus order-by-order the wavefunction, along with other properties, may be derived essentially analytically.

Since the perturbation parameter is the dimensionality of space and not the interaction, this approach is equally applicable to weakly interacting systems for which the mean-field approach is valid, and, perhaps more interestingly, strongly interacting systems for which the mean-field approach breaks down. Reference [1] extends previous work [21, 22, 27, 28] which derived energies, frequencies, normal-mode coordinates, wavefunctions and density profiles at lowest order for quantum systems of confined, interacting particles of any number, N.

The general formalism set forth in [1] for the wavefunction through first order, while essentially analytic, has many moving parts, and so this paper sets out to verify the formalism by applying it to the harmonically confined system of N particles interacting via harmonic potentials which may be attractive or repulsive. This system is exactly soluble in D dimensions, from which we directly derived the dimensional expansion for the wavefunction through first order in terms of the binary invariants. This expansion, directly from the exact wavefunction, has been compared with the wavefunction through first order from the general formalism of [1]. Since at each order there are only a finite number of binary invariants to consider, there are only a finite number of coefficients to the binary invariant terms that have to be compared. Exact agreement is found between the coefficients obtained directly from the independent solution and those derived using the general formalism of [1], confirming this general formalism.

The formalism of [1] is not limited to the harmonic interactions discussed in this paper, and indeed is quite general. In previous papers we have examined other potentials, in particular the hard-sphere potential in relation to Bose–Einstein condensates, at lowest order. While the lowest-order formalism adequately captures the behavior of the system in a range of scattering length, a, and particle number N for which the mean field is no longer an accurate description, for large enough a and/or N the lowest-order wavefunction no longer has the flexibility to adequately represent the actual system. [22] It is thus desirable to apply the general formalism of [1] for the wavefunction, through first order and verified in this paper, to other systems such as the Bose–Einstein condensate for interaction strengths and particle number at which the mean field breaks down.

In principle any observable quantity can be obtained from the wavefunction and as an illustration in [22] we derived the density profile at lowest order from the lowest-order wavefunction. With the next-order wavefunction available from the formalism of [1] we can now derive any observable quantity, such as the density profile, to next order in the perturbation theory. It is also important to note that while Laing *et al* [1] derive the *N*-particle wavefunction to next order in perturbation theory, the same basic approach can, in principle, be used to derive yet higher-order terms in the perturbation series.

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# Appendix. Confined, harmonically interacting, analytically solvable model system

In this appendix we derive the exact ground-state wavefunction for a harmonically confined, harmonically interacting system of N particles in D dimensions, and from it derive the wavefunction through first order in  $\delta^{1/2}$  exactly, where  $\delta = 1/D$ .

The Hamiltonian of the harmonically interacting model system of identical particles is

$$H = \frac{1}{2} \left( \sum_{i}^{N} \left[ -\frac{\partial^2}{\partial r_i^2} + \omega_t^2 r_i^2 \right] + \sum_{i < j}^{N} \omega_p^2 r_{ij}^2 \right).$$
(A.1)

Making the orthogonal transformation to center of mass and Jacobi coordinates

$$\boldsymbol{R} = \frac{1}{\sqrt{N}} \sum_{k=1}^{N} \boldsymbol{r}_{k} \quad \text{and} \quad \boldsymbol{\rho}_{i} = \frac{1}{\sqrt{i(i+1)}} \left( \sum_{j=1}^{i} \boldsymbol{r}_{j} - i \boldsymbol{r}_{i+1} \right), \quad (A.2)$$

where  $1 \leq i \leq N - 1$ , the Hamiltonian becomes

$$H = \frac{1}{2} \left( -\frac{\partial^2}{\partial \mathbf{R}^2} + \omega_t^2 \mathbf{R}^2 \right) + \frac{1}{2} \sum_{i=1}^{N-1} \left( -\frac{\partial^2}{\partial \rho_i^2} + \omega_{\text{int}}^2 \rho_i^2 \right), \tag{A.3}$$

the sum of N, D-dimensional harmonic-oscillator Hamiltonians, where

$$\omega_{\rm int} = \sqrt{\omega_t^2 + N\omega_p^2}.\tag{A.4}$$

Note two things about the Hamiltonian: it is separable and each component has the form of a *D*-dimensional harmonic oscillator. Therefore the ground-state solution to the wavefunction in the Schrödinger equation

$$H\Psi = E\Psi \tag{A.5}$$

is the product of harmonic-oscillator wavefunctions

$$\Psi(\boldsymbol{R}, \{\boldsymbol{\rho}_i\}; D) = \psi(\boldsymbol{R}; \omega_t, D) \prod_{i=1}^{N-1} \psi(\rho_i; \omega_{\text{int}}, D),$$
(A.6)

where  $\psi(\rho_i; \omega_{int}, D)$  is the D-dimensional, harmonic-oscillator, ground-state wavefunction

$$\psi(r;\omega,D) = \sqrt{\frac{2\omega^{\frac{D}{2}}}{\Gamma(\frac{D}{2})}} \exp\left(-\frac{\omega}{2}r^2\right)$$
(A.7)

satisfying the normalization condition

$$\int_0^\infty [\psi(r;\omega,D)]^2 r^{D-1} \, \mathrm{d}r = 1.$$
 (A.8)

The Jacobian-weighted, L = 0 wavefunction  $\Psi_J$  is obtained by folding into the wavefunction, the square root of that portion of the Jacobian which depends on the internal coordinates, i.e. the square root of

$$\Gamma^{(D-N-1)/2} \prod_{j=1}^{N} r_j^{(D-1)}, \tag{A.9}$$

where  $\Gamma$  is the Grammian determinant, so that

$$\Psi_J = \mathcal{N}\Gamma^{(D-N-1)/4} \prod_{j=1}^N r_j^{(D-1)/2} \psi(R; \omega_t, D) \prod_{i=1}^{N-1} \psi(\rho_i; \omega_{\text{int}}, D), \qquad (A.10)$$

where  $\mathcal{N}$  is a normalization constant ensuring that

$$\int [\Psi_J(\{r_i\}, \{\gamma_{jl}\}; D)]^2 \prod_i dr_i \prod_{j < k} d\gamma_{jk} = 1.$$
(A.11)

# A.1. A perturbation series in $1/\sqrt{D}$ for the exact wavefunction

A.1.1. Dimensional scaling. Now consider transforming to dimensionally scaled oscillator coordinates = 2

$$r = D^{2}\bar{a}_{t}\bar{r} \qquad \rho = D^{2}\bar{a}_{t}\bar{\rho} \qquad R = D^{2}\bar{a}_{t}\bar{R}$$

$$= \frac{D^{2}\bar{r}}{\sqrt{\bar{\omega}_{t}}} \qquad = \frac{D^{2}\bar{\rho}}{\sqrt{\bar{\omega}_{t}}} \qquad = \frac{D^{2}\bar{R}}{\sqrt{\bar{\omega}_{t}}} \qquad (A.12)$$

$$= \frac{D^{1/2}\bar{r}}{\sqrt{\omega_{t}}} \qquad = \frac{D^{1/2}\bar{\rho}}{\sqrt{\omega_{t}}} \qquad = \frac{D^{1/2}\bar{R}}{\sqrt{\omega_{t}}},$$

where the  $\omega_t = \frac{\bar{\omega}_t}{D^3}$ , and  $\bar{a}_t$  is the dimensionally scaled oscillator length of the trap. Both  $\bar{r}$  and  $\bar{\rho}$  are dimensionless. From equation (A.10) we obtain

$$\Psi_{J} = \mathcal{N}\Gamma^{(D-N-1)/4} \prod_{j=1}^{N} \bar{r}_{j}^{(D-1)/2} \sqrt{\frac{2}{\Gamma(\frac{D}{2})}} D^{\frac{D}{4}} \exp\left(-\frac{D}{2}\bar{R}^{2}\right) \\ \times \left(\frac{2}{\Gamma(\frac{D}{2})}\right)^{\frac{N-1}{2}} \left[ (\lambda D)^{\frac{D}{2}} \right]^{\frac{N-1}{2}} \prod_{i=1}^{N-1} \exp\left(-\frac{\lambda D}{2}\bar{\rho}_{i}^{2}\right), \tag{A.13}$$

where

$$\lambda = \frac{\omega_{\text{int}}}{\omega_t}.\tag{A.14}$$

A.1.2. The large-dimension limit. To test the general formalism of [1] we need to expand equation (A.13) about the large-dimension limit through first order in  $\delta^{1/2}$ . In the large-dimension limit the system localizes about a structure where all the radii are equal to  $\bar{r}_{\infty}$  and angle cosines are equal to  $\gamma_{\infty}$ . To derive  $\bar{r}_{\infty}$  and  $\gamma_{\infty}$  one applies the condition

$$\frac{\partial \Psi_J}{\partial \bar{r}_i}\Big|_{D=\infty} = \left.\frac{\partial \Psi_J}{\partial \gamma_{jk}}\right|_{D=\infty} = 0.$$
(A.15)

In this endeavor the following results are useful:

$$\Gamma|_{D=\infty} = (1 + (N-1)\gamma_{\infty})(1 - \gamma_{\infty})^{N-1},$$
(A.16)

$$\frac{\partial \Gamma}{\partial \gamma_{jk}}\Big|_{D=\infty} = -2\gamma_{\infty}(1-\gamma_{\infty})^{N-2}, \tag{A.17}$$

$$\bar{P}^{2}_{jk} = \bar{r}^{2}_{jk}(1+(N-1)); , \qquad (A.18)$$

$$\bar{R}^{2}|_{D=\infty} = \bar{r}_{\infty}^{2} (1 + (N - 1)\gamma_{\infty}),$$

$$\partial \bar{R}^{2}|_{(1 + (N - 1)\gamma_{\infty})}$$
(A.18)

$$\frac{\partial R}{\partial \bar{r}_i}\Big|_{D=\infty} = 2\bar{r}_\infty \frac{(1+(1+1)\bar{r}_\infty)}{N},\tag{A.19}$$

$$\left. \frac{\partial R^2}{\partial \gamma_{jk}} \right|_{D=\infty} = 2 \frac{\bar{r}_{\infty}^2}{N},\tag{A.20}$$

$$\sum_{i=1}^{N-1} \bar{\rho}_i^2 = \sum_{j=1}^N \bar{\rho}_j^2 - \bar{R}^2, \tag{A.21}$$

$$\sum_{i=1}^{N-1} \bar{\rho}_i^2 \bigg|_{D=\infty} = (N-1)\bar{r}_{\infty}^2 (1-\gamma_{\infty}) = (N-1)\bar{\rho}_{\infty},$$
(A.22)

$$\frac{\partial \sum_{i=1}^{N-1} \bar{\rho}_i^2}{\partial r_k} \bigg|_{D=\infty} = \frac{2(N-1)}{N} \bar{r}_{\infty} (1-\gamma_{\infty}), \tag{A.23}$$

$$\frac{\partial \sum_{i=1}^{N-1} \bar{\rho}_i^2}{\partial \gamma_{jk}} \bigg|_{D=\infty} = -\frac{2}{N} \bar{r}_{\infty}^2.$$
(A.24)

From equation (A.15) we obtain the parameters  $\bar{r}_{\infty}$  and  $\gamma_{\infty}$ 

$$\gamma_{\infty} = \frac{(\lambda - 1)}{(N + (\lambda - 1))},\tag{A.25}$$

$$\bar{r}_{\infty}^{2} = \frac{1}{2(1 + (N - 1)\gamma_{\infty})} = \frac{N + (\lambda - 1)}{2\lambda N}.$$
(A.26)

Equations (A.25) and (A.26) define the  $D \rightarrow \infty$  structure about which the system oscillates at finite dimension.

A.1.3. A series expansion about the large-D limit. To derive the wavefunction through order  $\delta^{1/2}$  we perform a series expansion of each of the D-dependent terms in equation (A.13).

$$\sqrt{\frac{1}{\Gamma\left(\frac{D}{2}\right)}} = \frac{2^{\frac{D-2}{4}}\exp\left(\frac{D}{4}\right)}{\sqrt[4]{\pi}D^{\frac{D-1}{4}}} + O(\delta),\tag{A.27}$$

$$\prod_{i=1}^{N} \bar{r}_{i}^{\frac{D-1}{2}} = \bar{r}_{\infty}^{\frac{N(D-1)}{2}} \exp\left(\sum_{i=1}^{N} \frac{D^{\frac{1}{2}} \bar{r}_{i}'}{2\bar{r}_{\infty}}\right) \exp\left(-\frac{1}{4\bar{r}_{\infty}^{2}} \sum_{i=1}^{N} \bar{r}_{i}'^{2}\right) \left(1 + \frac{\delta^{\frac{1}{2}}}{2} \sum_{i=1}^{N} \left(\frac{\bar{r}_{i}'^{3}}{3\bar{r}_{\infty}^{3}} - \frac{\bar{r}_{i}'}{\bar{r}_{\infty}}\right) + O(\delta)\right).$$
(A.28)

We also have

$$\bar{R}^2 = \bar{R}_{\infty}^2 + \delta^{1/2} \bar{R}_2'(\delta^{1/2}) \tag{A.29}$$

$$\sum_{i=1}^{N-1} \bar{\rho}_i^2 = (N-1)\bar{\rho}_{\infty}^2 + \delta^{1/2}{}_{\Sigma}\bar{\rho}_2'(\delta^{1/2}), \tag{A.30}$$

where

$$\bar{R}^{2}|_{D \to \infty} \equiv \bar{R}_{\infty}^{2} = \bar{r}_{\infty}^{2} (1 + (N - 1)\gamma_{\infty}),$$
(A.31)

$$\sum_{i=1}^{N-1} \bar{\rho}_i^2 \bigg|_{D \to \infty} \equiv (N-1)\bar{\rho}_{\infty}^2 = (N-1)\bar{r}_{\infty}^2 (1-\gamma_{\infty})$$
(A.32)

and

$$\bar{R}_{2}'(\delta^{1/2}) = \frac{2\bar{r}_{\infty}}{N} \left( (1 + (N - 1)\gamma_{\infty}) \sum_{i=1}^{N} \bar{r}_{i}' + \sum_{i< j=1}^{N} \bar{r}_{\infty} \bar{\gamma}_{ij}' \right) \\ + \frac{\delta^{1/2}}{N} \left( \sum_{i=1}^{N} (\bar{r}_{i}')^{2} + 2\gamma_{\infty} \sum_{i< j=1}^{N} \bar{r}_{i}' \bar{r}_{j}' + 2\bar{r}_{\infty} \sum_{i< j=1}^{N} (\bar{r}_{i}' + \bar{r}_{j}') \bar{\gamma}_{ij}' \right) + \delta \frac{2}{N} \sum_{i< j=1}^{N} \bar{r}_{i}' \bar{r}_{j}' \bar{\gamma}_{ij}',$$
(A.33)

$$\sum_{\Sigma} \bar{\rho}'_{2}(\delta^{1/2}) = \frac{2\bar{r}_{\infty}}{N} \left( (N-1)(1-\gamma_{\infty}) \sum_{i=1}^{N} \bar{r}'_{i} - \sum_{i< j=1}^{N} \bar{r}_{\infty} \bar{\gamma}'_{ij} \right)$$

$$+ \frac{\delta^{1/2}}{N} \left( (N-1) \sum_{i=1}^{N} (\bar{r}'_{i})^{2} - 2\gamma_{\infty} \sum_{i< j=1}^{N} \bar{r}'_{i} \bar{r}'_{j} - 2\bar{r}_{\infty} \sum_{i< j=1}^{N} (\bar{r}'_{i} + \bar{r}'_{j}) \bar{\gamma}'_{ij} \right)$$

$$- \delta \frac{2}{N} \sum_{i< j=1}^{N} \bar{r}'_{i} \bar{r}'_{j} \bar{\gamma}'_{ij},$$
(A.34)

so that

$$\exp\left(-\frac{D}{2}\bar{R}^{2}\right)\prod_{i=1}^{N-1}\exp\left(-\frac{\lambda D}{2}\bar{\rho}_{i}^{2}\right)$$

$$=\exp\left(-\frac{DN}{4}\right)\exp\left(-\sum_{i=1}^{N}\frac{D^{\frac{1}{2}}\bar{r}_{i}'}{2\bar{r}_{\infty}}\right)\exp\left(-\frac{D^{\frac{1}{2}}\bar{r}_{\infty}^{2}}{N}(1-\lambda)\sum_{i

$$\times\exp\left(-\frac{1}{2}\left(\left(\lambda-\frac{\lambda-1}{N}\right)\sum_{i=1}^{N}\bar{r}_{i}'^{2}-\frac{2(\lambda-1)}{N}\gamma_{\infty}\sum_{i

$$-\frac{2(\lambda-1)}{N}\bar{r}_{\infty}\sum_{i

$$\times\left(1+\delta^{\frac{1}{2}}\left(\frac{\lambda-1}{N}\right)\sum_{i
(A.35)$$$$$$$$

The final bit of the puzzle in the dimensional expansion of equation (A.13) is the dimensional expansion of  $\Gamma^{(D-N-1)/4}$ . For this we need equations (A.16), (A.17) and

$$\frac{\partial^2 \Gamma}{\partial \gamma_{ij} \partial \gamma_{kl}} \bigg|_{D=\infty} = 0, \tag{A.36}$$

$$\frac{\partial^2 \Gamma}{\partial \gamma_{ij} \partial \gamma_{jk}} \bigg|_{D=\infty} = 2\gamma_{\infty} (1 - \gamma_{\infty})^{N-3}, \tag{A.37}$$

$$\frac{\partial^2 \Gamma}{\partial \gamma_{ij}^2} \bigg|_{D=\infty} = -2(1 + (N-3)\gamma_{\infty})(1-\gamma_{\infty})^{N-3},$$
(A.38)

$$\left. \frac{\partial^3 \Gamma}{\partial \gamma_{ij} \partial \gamma_{kl} \partial \gamma_{mn}} \right|_{D=\infty} = 0, \tag{A.39}$$

$$\frac{\partial^3 \Gamma}{\partial \gamma_{ij} \partial \gamma_{jk} \partial \gamma_{lm}} \bigg|_{D=\infty} = 0, \tag{A.40}$$

$$\frac{\partial^{3}\Gamma}{\partial\gamma_{ij}\partial\gamma_{jk}\partial\gamma_{kl}}\Big|_{D=\infty} = -2\gamma_{\infty}(1-\gamma_{\infty})^{N-4}, \tag{A.41}$$

$$\frac{\partial^3 \Gamma}{\partial \gamma_{ij} \partial \gamma_{jk} \partial \gamma_{jl}} \bigg|_{D=\infty} = 0, \tag{A.42}$$

$$\frac{\partial^{3}\Gamma}{\partial\gamma_{ij}\partial\gamma_{jk}\partial\gamma_{ik}}\Big|_{D=\infty} = 2(1+(N-4)\gamma_{\infty})(1-\gamma_{\infty})^{N-4},$$
(A.43)

$$\left. \frac{\partial^3 \Gamma}{\partial \gamma_{ij}^2 \partial \gamma_{kl}} \right|_{D=\infty} = 4\gamma_\infty (1-\gamma_\infty)^{N-4},\tag{A.44}$$

$$\left. \frac{\partial^3 \Gamma}{\partial \gamma_{ij}^2 \partial \gamma_{jk}} \right|_{D=\infty} = 0, \tag{A.45}$$

$$\frac{\partial^3 \Gamma}{\partial \gamma_{ij}^3} \bigg|_{D=\infty} = 0, \tag{A.46}$$

from which we obtain

$$\begin{split} \Gamma^{(D-N-1)/4} &= \left( (1-\gamma_{\infty})^{N-1} (1+(N-1)\gamma_{\infty}) \right)^{\frac{D-N-1}{4}} \\ &\times \left( 1 + \frac{\delta^{\frac{1}{2}}}{12(1-\gamma_{\infty})(1+(N-1)\gamma_{\infty})} \left( -\frac{8\gamma_{\infty}^{3}}{(1-\gamma_{\infty})^{2}(1+(N-1)\gamma_{\infty})^{2}} [B(\rightarrow)\bar{\gamma}']^{3} \right) \\ &- \frac{6\gamma_{\infty}}{(1-\gamma_{\infty})^{2}(1+(N-1)\gamma_{\infty})} [B(\rightarrow)\bar{\gamma}'] \\ &\times \left\{ (1+(N-3)\gamma_{\infty})B(\bigcirc) - \gamma_{\infty}B(\bigcirc) \right\} \bar{\gamma}'\bar{\gamma}' \\ &+ \frac{1}{(1-\gamma_{\infty})^{2}} \left\{ (1+(N-4)\gamma_{\infty})B(\bigcirc) - \gamma_{\infty}B(\bigcirc) + 2\gamma_{\infty}B(\bigcirc) \right\} \bar{\gamma}'\bar{\gamma}'\bar{\gamma}' \\ &+ 6(N+1)\gamma_{\infty} [B(\rightarrow)\bar{\gamma}'] \right\} + O(\delta) \right) \exp\left( -D^{\frac{1}{2}} \frac{(\lambda-1)\bar{r}_{\infty}^{2}}{N} \sum_{i(A.47)$$

where  $[B(\mathcal{G})]_{\nu_1,\nu_2,\ldots}$  are the binary invariants introduced in [1] (briefly reviewed in appendix III) and  $\mathcal{G}$  is the graph labeling the binary invariant. The expression  $B(\mathcal{G})\bar{X}_1'\bar{X}_2'\bar{X}_3'$  is shorthand for  $[B(\mathcal{G})]_{\nu_1,\nu_2,\nu_3}[\bar{X}_1']_{\nu_1}[\bar{X}_2']_{\nu_2}[\bar{X}_3']_{\nu_2}$  where repeated indices  $\nu_i$  are summed over,  $\bar{X}'$  is the  $\bar{r}'$  or  $\bar{\gamma}'$  vector from equation (6), likewise for  $B(\mathcal{G})\bar{X}_1'\bar{X}_2'$  and  $B(\mathcal{G})\bar{X}_1'$ . Using equations (A.27), (A.28), (A.35) and (A.47), along with

$$B(\longrightarrow) \otimes B(\longrightarrow) = B(\bigcirc) + B(\bigcirc) + B(\longleftrightarrow)$$
(A.48)

$$B(\longrightarrow) \otimes B(\longrightarrow) \otimes B(\longrightarrow) = B(\bigoplus) + B(\swarrow) + B(\bigoplus) +$$

$$B(\to) \otimes B(\bigcirc) = B(\bigcirc) + \frac{B(\bigcirc \to)}{3} + \frac{B(\bigcirc}{3})$$
(A.50)

$$B(\longrightarrow) \otimes \frac{B(\square)}{2} = \frac{B(\bigcirc)}{3} + \frac{B(\square)}{2} + \frac{B(\square)}{2} + \frac{B(\square)}{3} + \frac{B(\square)}{6}$$
(A.51)

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in equation (A.13), with

$$\mathcal{N} = \frac{1}{\bar{r}_{\infty}^{\frac{N(D-1)}{2}} \left( (1 - \gamma_{\infty})^{N-1} (1 + (N-1)\gamma_{\infty}) \right)^{\frac{D-N-1}{4}}} + O(\delta),$$
(A.52)

we obtain the Jacobian-weighted *N*-body wavefunction in equation (25) for a system of identical particles under harmonic confinement with harmonic interactions.

#### References

- [1] Laing W, Dunn M and Watson D 2009 J. Math. Phys. at press (arXiv:math-ph/0808.2949v1)
- [2] Liu Y, Christandl M and Verstraete F 2007 Phys. Rev. Lett. 98 110503
- [3] Montina A 2008 Phys. Rev. A 77 22104
- [4] Masiello D, McKagan S and Reinhardt W 2005 Phys. Rev. A 72 63624
- [5] Cederbaum L S, Alon O E and Streltsov A I 2006 Phys. Rev. A 73 043609
- [6] Streltsov A, Alon O and Cederbaum L 2006 Phys. Rev. A 73 063626
- [7] Reynolds P J, Ceperley D M, Alder B J and Lester Jr W A 1982 J. Chem. Phys. 77 5593
- [8] Hammond B L, Lester W A Jr and Reynolds P J 1994 Monte Carlo Methods in ab initio Quantum Chemistry (Singapore: World Scientific)
- Bressanini D and Reynolds P J 1999 Advances in Chemical Physics: Monte Carlo Methods in Chemical Physics vol 105 ed D M Ferguson, J I Siepmann and D G Truhlar (New York: Wiley) pp 37–64
- [10] DuBois J L and Glyde H R 2001 Phys. Rev. A 63 023602
- [11] DuBois J L and Glyde H R 2003 Phys. Rev. A 68 033602
- [12] Purwanto W and Zhang S 2005 Phys. Rev. A 72 053610
- [13] Landau D and Binder K 2001 A Guide to Monte-Carlo Simulations in Statistical Physics (Cambridge: Cambridge University Press)
- [14] Holzmann M, Krauth W and Naraschewski M 1999 Phys. Rev. A 59 2956
- [15] Nilsen J K, Mur-Petit J, Guilleumas M, Hjorth-Jensen M and Polls A 2005 Phys. Rev. A 71 053610
- [16] Blume D and Greene C H 2001 *Phys. Rev.* A **63** 63061
- [17] Minguzzi A, Succi S, Toschi F, Tosi M and Vignolo P 2004 Phys. Rep. 395 223
- [18] Nunes G S 1999 J. Phys. B: At. Mol. Opt. Phys. 32 4293
- [19] Banerjee A and Singh M P 2001 Phys. Rev. A 64 063604
- [20] Gasenzer T, Berges J, Schmidt M and Seco M 2005 Phys. Rev. A 72 63604
- [21] Dunn M, Watson D and Loeser J 2006 Ann. Phys. (NY) 321 1939
- [22] Laing W B, Dunn M and Watson D K 2006 Phys. Rev. A 74 063605
- [23] Laing W B, Dunn M, Loeser J G and Watson D K 2005 arXiv:physics/0510177v1
- [24] Gross J L and Yellen J (eds) 2004 Handbook of Graph Theory (Boca Raton, FL: CRC Press)
- [25] Laing W B, Dunn M and Watson D K 2009 at press (http://nhn.ou.edu/~watson/papers/jmp08/EPAPSlaing08.pdf)

Laing W B, Dunn M and Watson D K EPAPS electronic depository, see http://www.aip.org/pubservs/epaps.html (submitted)

- [26] Kelle D 2008 Binary invariants are a basis, unpublished
- [27] McKinney B, Dunn M, Watson D and Loeser J 2003 Ann. Phys. (NY) 310 56
- [28] McKinney B, Dunn M and Watson D 2004 Phys. Rev. A 69 053611
- [29] Wolfram Research 2007 Mathematica edition: Version 6.0