Test of a general symmetry-derived *N*-body wave function

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The resources required to solve the general interacting quantum *N*-body problem scale exponentially with *N*, making the solution of this problem very difficult when *N* is large. In a previous series of papers we develop an approach for a fully interacting wave function for a confined system of identical bosons with a general two-body interaction. This method tames the *N* scaling by developing a perturbation series that is order-by-order invariant under a point group isomorphic with S_N. Group theory and graphical techniques are then used to solve for the wave function exactly and analytically at each order, yielding a solution for the general *N*-body problem which scales as N^0 at any given order. Recently this formalism has been used to obtain the first-order fully interacting wave function for a system of harmonically confined bosons interacting harmonically. In this paper, we report the application of this *N*-body wave function to a system of *N* fully interacting bosons in three dimensions. We derive an expression for the density profile for a confined system of harmonically interacting bosons. Choosing this simple interaction is not necessary or even advantageous for our method, however this choice allows a direct comparison of our exact results through first order with exact results obtained in an independent solution. Our density profile for the wave function through first order in three dimensions is indistinguishable from the first-order exact result obtained independently and shows strong convergence to the exact result to all orders.

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I. INTRODUCTION

The interacting quantum *N*-body problem becomes particularly challenging when *N* is large. Unlike the corresponding classical problem where the resources required to solve the problem scale as a polynomial in *N*, the resources needed to solve the quantum *N*-body problem scale exponentially with *N*, frequently doubling for every particle added [1,2]. When interparticle interactions are weak, the mean-field approximation may be used to avoid this exponential scaling with *N*. When interactions are larger, phenomenological models are often used. Typically the phenomenological models are only valid for a range of interaction strengths, masses, etc., so more general first-principles approaches which tackle the quantum mechanical exponential *N*-scaling issue head on are needed [3,4]. Such first-principles methods for confined *N*-particle quantum systems include coupled cluster methods [5], the method of correlated basis functions [6,7], and density functional theory [8]. Of particular note in this regard are Monte Carlo methods [3,4,9–18].

We take a different approach and develop a non-numerical method for systems of confined identical bosons which uses group theory and graphical techniques to tackle the *N*-scaling problem (see Ref. [19] and the references therein). This method circumvents the severity of the *N*-scaling problem by using a perturbation expansion about a maximally symmetric structure in large dimensions which has a point group isomorphic to S_N. Group theory is then used to separate the *N* scaling problem away from the interaction dynamics, allowing the *N* scaling to be treated as a straight mathematical issue. The perturbation expansion of the Hamiltonian is order-by-order invariant under the S_N point group, yielding a problem at each perturbation order that can be solved, essentially exactly and analytically, using group theory and graphical techniques. 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 scales as N^0.

As part of this solution, small finite, S_N-invariant basis sets are used that are complete at each order, and as *N* increases, the group theory and graphical techniques "hold their own" with the result that the number of elements of this basis does not grow with *N*. (The basis elements must remain invariant under the *N*! operations of the S_N group which puts increasing restrictions on the growth of the set as *N* gets larger.) The completeness of this basis at each order was established in Ref. [19]. Since the elements of this basis, called binary invariants, are themselves invariant under the maximal point group symmetry, the invariance of the Hamiltonian at each order is naturally ensured by expressing it in terms of this relatively small basis (7 elements at lowest order in the wave function and 25 elements at next order).

The equation for the lowest-order wave function is solved by a transformation to normal coordinates. At first this would seem to be a formidable task since there are $N(N+1)$ coordinates to transform into normal coordinates. However, this transformation is facilitated analytically, for arbitrary *N*, by the fact that the large-dimension S_N point group symmetry greatly reduces the size of the basis to only seven members at this order for any *N*.

Applying this approach at lowest order, we have previously derived beyond-mean-field energies [20,21], frequencies [20], normal mode coordinates [22], wave functions [22], and density profiles [23] for general isotropic interacting confined quantum systems (a brief four page summary of

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the method at lowest order, along with some lowest-order results, may be found in Ref. [24]). More recently, in a major development of the method presented in Refs. [19,25], we have extended this analysis to first order in the wave function, which required the development of new techniques to handle, exactly and analytically, the complexity of coupling the many normal coordinates of the lowest-order solution. This basic approach, developed at first order, is general enough to be extended to higher orders in the perturbation expansion. In Ref. [19], the general theory in Ref. [25], which derives the wave function through first order for an arbitrary isotropic system, was tested on the exactly soluble system of N harmonically interacting particles under harmonic confinement. When this wave function was compared to the exact analytic wave function obtained in an independent solution and then expanded analytically through first order, exact agreement was found, confirming this general theory for a fully interacting N-body system in three dimensions [19].

In the present paper, we test this general fully interacting wave function in Ref. [25], exact through first order, by deriving a property—namely, the density profile which is directly observable in the laboratory for a Bose-Einstein condensate (BEC). We test it on the same exactly soluble system of N harmonically interacting particles under harmonic confinement. Our density profile analytically derived from the first-order wave function and evaluated at $D=3$ is indistinguishable from the $D=3$ first-order result from the independent solution and shows strong convergence to the exact $D=3$ result to all orders.

This derivation of the density profile for the wave function through first order builds upon previous isotropic work. The isotropic lowest-order ground-state wave function was derived in Ref. [22] and the corresponding lowest-order ground-state density profile was derived from this in Ref. [23]. The isotropic *first-order* ground-state wave function was derived in Ref. [25] and checked in Ref. [19]. This work is reviewed in Sec. II. The derivation of the density profile for the general wave function through first order is found in Sec. III. Section IV presents the application and results. The Appendix presents the exact independent solution for the density profile through first order from the full D-dimensional density profile for this system, which is also derived independently in the Appendix from the full D-dimensional wave function for the harmonically interacting system discussed in Ref. [19]. Section V is the summary and conclusions section.

II. DIMENSIONAL EXPANSION AND LARGE-DIMENSION POINT GROUP SYMMETRY

A. Dimensionally scaled Jacobian-weighted *S*-wave Hamiltonian in internal coordinates

In previous papers we have been developing an approach to the quantum mechanical problem of N interacting particles confined by an external potential, where N may be less than 10 to 10^7 or larger. This approach uses the inverse dimensionality of space as an expansion parameter. Both the lowest-order and first-order wave functions have been derived, as well as the lowest-order density profile and corresponding energy [19–23,25,26].

In dimensionally scaled oscillator units, the Jacobian weighted, $L=0$ Schrödinger equation reads [23,27]

$$\bar{H}\Phi = \left(\frac{1}{\kappa(D)}\bar{T} + \bar{V}_{\rm eff}\right)\Phi = \bar{E}\Phi, \tag{1}$$

where

$$\bar{T} = \hbar^2\left[-\sum_{i=1}^{N}\frac{1}{2m_i}\frac{\partial^2}{\partial \bar{r}_i^2} - \sum_{i=1}^{N-1}\frac{1}{2m_i\bar{r}_i^2}\sum_{j>i}^{N}\sum_{k>i}^{N}\frac{\partial}{\partial\gamma_{ij}}\frac{(\gamma_{jk}-\gamma_{ij}\gamma_{ik})}{4}\frac{\partial}{\partial\gamma_{ik}}\right], \tag{2}$$

γ_{ij} is the angle cosine between particle i and particle j,

$$\bar{r}_i = \frac{r_i}{\kappa(D)}, \quad \bar{E} = \kappa(D)E, \quad \bar{H} = \kappa(D)H, \tag{3}$$

r_i is the distance of particle i from the center of the confining potential, and $\kappa(D)$ is a dimensional scaling factor which regularizes the large-dimension limit (it is discussed in more detail below). The effective potential $\bar{V}_{\rm eff}$ is composed of the nonderivative ("centrifugal") portion of the kinetic energy $\bar{U}$ plus the confining and interparticle potentials, $\bar{V}_{\rm conf}$ and $\bar{V}$, respectively, i.e.,

$$\bar{V}_{\rm eff} = \bar{U} + \bar{V}_{\rm conf} + \bar{V}, \tag{4}$$

where

$$\bar{V}_{\rm conf} = \sum_{i=1}^{N}\bar{v}_{\rm conf}(\bar{r}_i), \tag{5}$$

$$\bar{U} = \sum_{i=1}^{N}\hbar^2\frac{N(N-2)+(D-N-1)^2\left(\frac{\Gamma^{(i)}}{\Gamma}\right)}{\kappa(D)8m_i\bar{r}_i^2}, \tag{6}$$

$$\bar{V} = \sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\bar{V}_{\rm int}(\bar{r}_{ij}), \tag{7}$$

Γ is the Gramian determinant, the determinant of the matrix whose elements are γ_{ij} (see Appendix D in Ref. [21]), and $\Gamma^{(i)}$ is the determinant of the same matrix minus the ith row and ith column. The $\lim_{D\to\infty}\kappa(D)\propto D^2$ to ensure that $\bar{U}$ is finite as $D\to\infty$. Defining δ to be the inverse dimensionality (so that $\lim_{D\to\infty}$ is equivalent to $\lim_{\delta\to 0}$) and $\zeta(\delta)$ to be the ratio of D^2 to $\kappa(D)$,

$$\delta = \frac{1}{D}, \tag{8}$$

$$\zeta(\delta) = \frac{1}{\delta^2\kappa(D)}, \tag{9}$$

then $\zeta(\delta)$ is finite as $\delta\to 0$ $(D\to\infty)$. The actual form of $\kappa(D)$ is chosen to simplify the problem at hand subject to the

requirement that $\lim_{D\to\infty}\kappa(D)\propto D^2$. Examples of $\kappa(D)$ for various systems are listed after Eq. (10) in Ref. [23].

Defining a position vector, $\bar{\boldsymbol{y}}$, consisting of all $N(N+1)/2$ internal coordinates,

$$\bar{\boldsymbol{y}}=\begin{pmatrix}\bar{\boldsymbol{r}}\\ \boldsymbol{\gamma}\end{pmatrix},\quad \text{where}\quad \boldsymbol{\gamma}=\begin{pmatrix}\gamma_{12}\\ \hline \gamma_{13}\\ \gamma_{23}\\ \hline \gamma_{14}\\ \gamma_{24}\\ \gamma_{34}\\ \hline \gamma_{15}\\ \gamma_{25}\\ \vdots\\ \gamma_{N-2,N}\\ \gamma_{N-1,N}\end{pmatrix}\quad\text{and}\quad \bar{\boldsymbol{r}}=\begin{pmatrix}\bar{r}_1\\ \bar{r}_2\\ \vdots\\ \bar{r}_N\end{pmatrix}, \tag{10}$$

and taking all of the masses of the particles to be the same, $m_i=m$, Eq. (1) can be written as

$$\bar{H}\Phi=[\delta^2\zeta(\delta)\bar{T}+\bar{V}_{\text{eff}}]\Phi=\bar{E}\Phi, \tag{11}$$

where

$$\zeta(\delta)\bar{T}=-\tfrac{1}{2}\partial_{\bar{y}_{\nu_1}}G(\bar{\boldsymbol{y}};\delta)_{\nu_1,\nu_2}\,\partial_{\bar{y}_{\nu_2}}, \tag{12}$$

$$\bar{V}_{\text{eff}}(\bar{\boldsymbol{y}};\delta,N)=\bar{U}(\bar{\boldsymbol{y}};\delta,N)+\bar{V}_{\text{conf}}(\bar{\boldsymbol{y}};\delta,N)+\bar{V}(\bar{\boldsymbol{y}};\delta,N), \tag{13}$$

$$\bar{U}(\bar{\boldsymbol{y}};\delta,N)=\sum_{i=1}^{N}\hbar^2\zeta(\delta)\frac{N(N-2)\delta^2+[1-(N+1)\delta]^2\left(\frac{\Gamma^{(i)}}{\Gamma}\right)}{8m\bar{r}_i^2}, \tag{14}$$

$\partial_{\bar{y}_\nu}=\partial/\partial\bar{y}_\nu$ are the derivatives of the elements of the $\bar{\boldsymbol{y}}$ column vector, and $\mathbf{G}(\bar{\boldsymbol{y}};\delta)$ is the $N(N+1)/2\times N(N+1)/2$ dimensional block-diagonal tensor,

$$\boldsymbol{G}(\bar{\boldsymbol{y}};\delta)=\left(\begin{array}{c|c}\frac{\hbar^2\zeta(\delta)}{m}\boldsymbol{I}_N & \boldsymbol{0}\\ \hline \boldsymbol{0} & \boldsymbol{G}^{\gamma\gamma}(\bar{\boldsymbol{r}},\boldsymbol{\gamma};\delta)\end{array}\right), \tag{15}$$

with $\boldsymbol{I}_N$ as the $N\times N$ dimensional diagonal unit tensor, $\boldsymbol{G}^{\gamma\gamma}(\bar{\boldsymbol{r}},\boldsymbol{\gamma};\delta)$ as the $N(N-1)/2\times N(N-1)/2$ dimensional matrix of elements,

$$[\boldsymbol{G}^{\gamma\gamma}(\bar{\boldsymbol{r}},\boldsymbol{\gamma};\delta)]_{(ij),(lk)}=\frac{\hbar^2\zeta(\delta)}{m}\frac{(\gamma_{jk}-\gamma_{ij}\gamma_{lk})}{4\bar{r}_i^2}\delta_{il}, \tag{16}$$

and δ_{il} is the Kronecker delta (as distinct from the inverse spatial dimension, δ). This paper uses the implicit summation convention, i.e., repeated indices are summed over (unless explicitly noted otherwise), and this convention has been used in Eq. (12).

B. Dimensional expansion

As discussed in previous papers, the Hamiltonian and Jacobian-weighted wave function and energy are expanded in powers of $\delta^{1/2}$, where $\delta=1/D$. Dimensionally scaled internal displacement coordinates, $\bar{r}_i'$ and $\bar{\gamma}_{ij}'$, are introduced,

$$\bar{r}_i=\bar{r}_\infty+\delta^{1/2}\bar{r}_i'\quad\text{and}\quad\gamma_{ij}=\gamma_\infty+\delta^{1/2}\bar{\gamma}_{ij}', \tag{17}$$

where the $\bar{r}_i$ are the dimensionally scaled radii and the γ_{ij} are the angle cosines between the position vectors of the N particles. They are collected together to form the internal displacement coordinate vector $\bar{y}_\nu'$ where

$$\bar{\boldsymbol{y}}'=\begin{pmatrix}r\\ \bar{\boldsymbol{\gamma}}'\end{pmatrix},\quad\text{where}\quad\bar{\boldsymbol{\gamma}}'=\begin{pmatrix}\bar{\gamma}_{12}'\\ \hline \bar{\gamma}_{13}'\\ \bar{\gamma}_{23}'\\ \hline \bar{\gamma}_{14}'\\ \bar{\gamma}_{24}'\\ \bar{\gamma}_{34}'\\ \hline \bar{\gamma}_{15}'\\ \bar{\gamma}_{25}'\\ \vdots\\ \bar{\gamma}_{N-2,N}'\\ \bar{\gamma}_{N-1,N}'\end{pmatrix}\quad\text{and}\quad\bar{\boldsymbol{r}}'=\begin{pmatrix}\bar{r}_1'\\ \bar{r}_2'\\ \vdots\\ \bar{r}_N'\end{pmatrix}, \tag{18}$$

and the dimensionally scaled, Jacobian-weighted Hamiltonian, Jacobian-weighted wave function and the dimensionally scaled energy are expanded in powers of $\delta^{1/2}$ to give

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

$$\Phi(\bar{r}_i,\gamma_{ij})=\sum_{j=0}^{\infty}(\delta^{1/2})^j\Phi_j,$$

$$\bar{E}=\bar{E}_\infty+\delta^{1/2}\bar{E}_{-1}+\delta\sum_{j=0}^{\infty}(\delta^{1/2})^j\bar{E}_j, \tag{19}$$

where

$$\bar{H}_\infty=\bar{E}_\infty, \tag{20}$$

$$\bar{H}_{-1}=\bar{E}_{2n-1}=0, \tag{21}$$

$$\bar{H}_0=-\tfrac{1}{2}\,{}^{(0)}_{2}G_{\nu_1,\nu_2}\partial_{\bar{y}_{\nu_1}'}\partial_{\bar{y}_{\nu_2}'}+\tfrac{1}{2}\,{}^{(0)}_{2}F_{\nu_1,\nu_2}\bar{y}_{\nu_1}'\bar{y}_{\nu_2}'+{}^{(0)}_{0}F, \tag{22}$$

$$\bar{H}_1=-\frac{1}{2}\,{}^{(1)}_{3}G_{\nu_1,\nu_2,\nu_3}\bar{y}_{\nu_1}'\partial_{\bar{y}_{\nu_2}'}\partial_{\bar{y}_{\nu_3}'}-\frac{1}{2}\,{}^{(1)}_{1}G_\nu\partial_{\bar{y}_\nu'}+\frac{1}{3!}\,{}^{(1)}_{3}F_{\nu_1,\nu_2,\nu_3}\bar{y}_{\nu_1}'\bar{y}_{\nu_2}'\bar{y}_{\nu_3}'+{}^{(1)}_{1}F_\nu\bar{y}_\nu'. \tag{23}$$

The superprescript on the $\boldsymbol{F}$ and $\boldsymbol{G}$ tensors in parentheses in Eqs. (21)–(23) denotes the order in $\delta^{1/2}$ that the term en-

ters (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 $\bar{\boldsymbol{y}}'$ (second order in the derivatives) and formed of either all even or all odd powers of the elements and derivatives of $\bar{\boldsymbol{y}}'$ when n is even or odd, respectively.

C. Large-dimension point group

According to Eq. (17) 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, equiangular from each other, and hence equidistant 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 frozen $D\to\infty$ structure. This together with the fact that the full D-dimensional Hamiltonian, $\hat{H}$, is invariant under particle exchange means the dimensional expansion of Eq. (19) is order-by-order invariant under this S_N point group, i.e., the $\bar{H}_j$ are each invariant under the S_N point group.

D. Normal mode coordinates and lowest-order wave function

According to Eq. (22), $\bar{H}_0$, which determines the lowest-order wave function, is that of a multidimensional harmonic oscillator, and so a solution for the lowest-order wave function is effected through a transformation to normal coordinates. Since $\bar{H}_0$ is invariant under the S_N point group, these normal modes transform under irreducible representations (irreps.) of the S_N group. The transformation to normal modes is linear, and so the irreps. which the normal modes transform under are determined by the irreps. present in the reducible representations under which the $\bar{\boldsymbol{r}}'$ and $\bar{\boldsymbol{\gamma}}'$ vectors transform. These are found to be the $[N]$, $[N-1,1]$, and $[N-2,2]$ irreps. Two normal modes transform under two one-dimensional $[N]$ irreps. of S_N, $2(N-1)$ normal modes transform under two $(N-1)$-dimensional $[N-1,1]$ irreps., and the $N(N-3)/2$ normal modes transform under an $N(N-3)/2$-dimensional $[N-2,2]$ irrep. We denote the two one-dimensional $[N]$ irreps. by $\mathbf{0}^+$ and $\mathbf{0}^-$, the two $(N-1)$-dimensional $[N-1,1]$ irreps. by $\mathbf{1}^+$ and $\mathbf{1}^-$, and the $N(N-3)/2$-dimensional $[N-2,2]$ irrep. by $\mathbf{2}$.

If the normal modes are chosen to transform under *orthogonal* $[N]$, $[N-1,1]$, and $[N-2,2]$ irreps. of S_N, then $\bar{H}_0$ takes the form

$$\bar{H}_0=-\tfrac{1}{2}\partial_{\boldsymbol{q}'}^T\partial_{\boldsymbol{q}'}+\tfrac{1}{2}\boldsymbol{q}'^T\boldsymbol{\Lambda}\boldsymbol{q}'+{}_0^{(0)}F, \tag{24}$$

where $\boldsymbol{\Lambda}$ is the diagonal matrix of the square of the frequencies. While there are $N(N+1)/2$ frequencies, one for each of the normal modes, the large-dimension S_N point group greatly limits the number of distinct frequencies to at most only *five*, one for each of the five sets of normal modes labeled by $\mathbf{0}^+$, $\mathbf{0}^-$, $\mathbf{1}^+$, $\mathbf{1}^-$, and $\mathbf{2}$.

From Eq. (24) the lowest-order wave function is a product of $N(N+1)/2$ one-dimensional harmonic-oscillator wave functions in the normal mode coordinates,

$$\Phi_0(\mathbf{q}')=\prod_{\mu=\{\mathbf{0}^\pm,\mathbf{1}^\pm,\mathbf{2}\}}\prod_{\xi=1}^{d_\mu}\phi_{n(\mu,\xi)}(\sqrt{\bar{\omega}_\mu}[q'_\mu]_\xi), \tag{25}$$

where $\phi_{n(\mu,\xi)}(\sqrt{\bar{\omega}_\mu}[q'_\mu]_\xi)$ is a one-dimensional harmonic-oscillator wave function of frequency $\bar{\omega}_\mu$ and $n(\mu,\xi)$ is the oscillator quantum number, $0\le n(\mu,\xi)<\infty$, which counts the number of quanta in each normal mode. The index μ labels the manifold of normal modes with the same frequency $\bar{\omega}_\mu$ while degeneracy of the μth normal mode is denoted $d_\mu=1$, $N-1$, or $N(N-3)/2$ for $\mu=\mathbf{0}^\pm$, $\mathbf{1}^\pm$, or $\mathbf{2}$, respectively.

E. Transformation to normal modes: Symmetry coordinates

The transformation to normal modes would appear to be a formidable proposition since if N is in the millions, the number of normal modes P is of the order 10^{12} or larger. However, the $D\to\infty$ structure is maximally symmetric (see Ref. [21]), and it is this maximal point group symmetry which allows the normal modes to be derived (see Ref. [22]).

The normal modes may be written as

$$\boldsymbol{q}'^{\alpha}_{\pm}=c^{\alpha}_{\pm}(\cos\,\theta^{\alpha}_{\pm}[\boldsymbol{S}^{\alpha}_{\bar{\boldsymbol{r}}'}]_\xi+\sin\,\theta^{\alpha}_{\pm}[\boldsymbol{S}^{\alpha}_{\bar{\boldsymbol{\gamma}}'}]_\xi) \tag{26}$$

for the $\alpha=[N]$ and $[N-1,1]$ sectors, where the $\pm$ denote the two normal mode vectors for each α and

$$\boldsymbol{q}'^{[N-2,2]}=c^{[N-2,2]}\boldsymbol{S}^{[N-2,2]}_{\bar{\boldsymbol{\gamma}}'}, \tag{27}$$

where the symmetry coordinates $[\boldsymbol{S}^{\alpha}_{X'}]_\xi$ (defined in Ref. [22]) may be written as

$$\mathbf{S}^{[N]}_{r'}=\frac{1}{\sqrt{N}}\sum_{k=1}^{N}\bar{r}'_k,\quad \mathbf{S}^{[N]}_{\gamma'}=\sqrt{\frac{2}{N(N-1)}}\sum_{l=2}^{N}\sum_{k=1}^{l-1}\bar{\gamma}'_{kl},$$

$$[\mathbf{S}^{[N-1,1]}_{r'}]_i=\frac{1}{\sqrt{i(i+1)}}\left(\sum_{k=1}^{i}\bar{r}'_k-i\bar{r}'_{i+1}\right),$$

$$[\mathbf{S}^{[N-1,1]}_{\gamma'}]_i=\frac{1}{\sqrt{i(i+1)(N-2)}}\left(\left[\sum_{l=2}^{i}\sum_{k=1}^{l-1}\bar{\gamma}'_{kl}+\sum_{k=1}^{i}\sum_{l=k+1}^{N}\bar{\gamma}'_{kl}\right]-i\left[\sum_{k=1}^{i}\bar{\gamma}'_{k,i+1}+\sum_{l=i+2}^{N}\bar{\gamma}'_{i+1,l}\right]\right),$$

where $1\le i\le N-1$, and

$$[\mathbf{S}^{[N-2,2]}_{\gamma'}]_{ij}=\frac{1}{\sqrt{i(i+1)(j-3)(j-2)}}\left[\sum_{j'=2}^{j-1}\sum_{k=1}^{[j'-1,i]_{min}}\bar{\gamma}'_{kj'}+\sum_{k=1}^{i-1}\sum_{j'=k+1}^{i}\bar{\gamma}'_{kj'}-(j-3)\sum_{k=1}^{i}\bar{\gamma}'_{kj}-i\left(\sum_{k=1}^{i}\bar{\gamma}'_{k,(i+1)}+\sum_{j'=i+2}^{j-1}\bar{\gamma}'_{(i+1),j'}\right)\right)$$

$$+ i(j-3)\bar{\gamma}'_{(i+1),j}\Bigg], \tag{28}$$

where $1 \le i \le j-3$ and $i+3 \le j \le N$.

F. Next-order Hamiltonian correction in the normal coordinate basis: Clebsch-Gordan coefficients of S_N

After applying the linear transformation to normal modes to the higher-order terms in the expansion of $\bar{H}$ in Eq. (19), each of the higher-order terms, $\bar{H}_j$, is polynomial in the normal modes and their derivatives. Defining G_V and F_V to be the G and F tensors in the normal coordinate basis, the first-order Hamiltonian takes the form

$$\bar{H}_1 = -\frac{1}{2}[{}^{(1)}_{3}G_V]_{\nu_1,\nu_2,\nu_3}\,\bar{q}'_{\nu_1}\partial_{\bar{q}'_{\nu_2}}\partial_{\bar{q}'_{\nu_3}} + \frac{1}{3!}[{}^{(1)}_{3}F_V]_{\nu_1,\nu_2,\nu_3}\,\bar{q}'_{\nu_1}\bar{q}'_{\nu_2}\bar{q}'_{\nu_3}$$
$$-\frac{1}{2}[{}^{(1)}_{1}G_V]_{\nu}\,\partial_{\bar{q}'_{\nu}} + [{}^{(1)}_{1}F_V]_{\nu}\,\bar{q}'_{\nu}. \tag{29}$$

Since each higher-order term is scalar under the maximal S_N point group symmetry i.e., they transform under the $[N]$ representation of the maximal S_N point group, the normal coordinates in each monomial term in $\bar{H}_j$ must be coupled together by Clebsch-Gordan coefficients of S_N to produce a scalar quantity. Thus we can write

$$[{}^{(1)}_{1}G_V]_{\nu} = [{}^{(1)}_{1}\tau^{G}_{[N]}]_{Y}\,\delta_{[N]\alpha},$$

$$[{}^{(1)}_{1}F_V]_{\nu} = [{}^{(1)}_{1}\tau^{F}_{[N]}]_{Y}\,\delta_{[N]\alpha},$$

$$[{}^{(1)}_{3}G_V]_{\nu_1,\nu_2,\nu_3} = \sum_{\mathcal{R}}[{}^{(1)}_{3}\tau^{G}_{\alpha_1,\alpha_2,\alpha_3,\mathcal{R}}]_{Y_1,Y_2,Y_3}\,[C^{\alpha_1\alpha_2\alpha_3,\mathcal{R}}]_{\xi_1,\xi_2,\xi_3},$$

$$[{}^{(1)}_{3}F_V]_{\nu_1,\nu_2,\nu_3} = \sum_{\mathcal{R}}[{}^{(1)}_{3}\tau^{F}_{\alpha_1,\alpha_2,\alpha_3,\mathcal{R}}]_{Y_1,Y_2,Y_3}\,[C^{\alpha_1\alpha_2\alpha_3,\mathcal{R}}]_{\xi_1,\xi_2,\xi_3}, \tag{30}$$

where the $\delta_{[N]\alpha}$ and $C^{\alpha_1\alpha_2\alpha_3,\mathcal{R}}$ are the appropriate Clebsch-Gordan coefficient of S_N. Here repeated α_1, α_2, and α_3 labels are *not* summed over. The indices Y run over + and −. There are two linearly independent Clebsch-Gordan coefficients coupling three $[N-2,2]$ irreps. together to form a scalar $[N]$ irrep. Thus $\mathcal{R}$ has two values, running from I to II when $\alpha_1\alpha_2\alpha_3 = \mathbf{222}$. All other couplings of the $[N]$, $[N-1,1]$, and $[N-2,2]$ irreps. have only one Clebsch-Gordan coefficient, and so $\mathcal{R}$ has only one value, I. The small coefficient tensors, τ, depend on the specifics of the system.

G. First-order wave function

Previous applications of dimensional expansions went to very high order, but for systems with a large number of degrees of freedom, the derivation of these high order terms is computationally prohibitive and subject to numerical difficulties. In Ref. [28] Dunn *et al.* presented an algorithm by which these corrections may be derived exactly using tensor algebra. Using this formalism, the first-order correction to the lowest-order wave function is derived in Ref. [25]. Writing the wave function through first order as

$$\Phi_1(\mathbf{q}') = (1 + \delta^{1/2}\hat{\Delta})\Phi_0(\mathbf{q}'), \tag{31}$$

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

$$[\hat{\Delta}, \bar{H}_0]\Phi_0 = \bar{H}_1\Phi_0. \tag{32}$$

To solve this equation, it is helpful to note that since $\Phi_0(\mathbf{q}')$ is a Gaussian function, the derivatives in $\bar{H}_1$ and $\bar{H}_0$ written in normal coordinates "bring down" normal coordinates from the exponent so that $\bar{H}_1$ effectively becomes a third-order polynomial of only odd powers in $\mathbf{q}'$.

1. Evaluation of derivatives in $\hat{H}_1\Phi_0$

We evaluate the derivatives implicit in Eq. (32), noting the Gaussian form of $\Phi_0(\mathbf{q}')$, to reduce the operator equation to a polynomial equation in q'_ν,

$$\partial_{q'_\nu}\Phi_0(\mathbf{q}') = -\bar{\omega}_\nu q'_\nu\,\Phi_0(\mathbf{q}'), \tag{33}$$

$$\partial^2_{q'_\nu}\Phi_0(\mathbf{q}') = [-\bar{\omega}_\nu + \bar{\omega}^2_\nu (q'_\nu)^2]\Phi_0(\mathbf{q}'). \tag{34}$$

Therefore with the substitutions

$$\partial_{q'_\nu} \to -\bar{\omega}_\nu q'_\nu, \tag{35}$$

$$\partial_{q'_{\nu_i}}\partial_{q'_{\nu_j}} \to \bar{\omega}_{\nu_i}\bar{\omega}_{\nu_j} q'_{\nu_i} q'_{\nu_j} - \delta_{ij}\,\bar{\omega}_{\nu_i}, \tag{36}$$

the action of $\bar{H}_1$ on $\Phi_0(\mathbf{q}')$ becomes equivalent to the action of a third-order polynomial $(\bar{H}_1)_{\text{eff}}$ on $\Phi_0(\mathbf{q}')$,

$$\bar{H}_1\Phi_0(\mathbf{q}') = (\bar{H}_1)_{\text{eff}}\,\Phi_0(\mathbf{q}'), \tag{37}$$

where

$$(\bar{H}_1)_{\text{eff}} = \sum_{\nu_1,\nu_2,\nu_3}\Bigg(-\frac{1}{2}[{}^{(1)}_{3}G_V]_{\nu_1,\nu_2,\nu_3}\,\bar{\omega}_{\nu_2}\bar{\omega}_{\nu_3}$$
$$+\frac{1}{3!}[{}^{(1)}_{3}F_V]_{\nu_1,\nu_2,\nu_3}\Bigg)q'_{\nu_1}q'_{\nu_2}q'_{\nu_3}$$
$$+\sum_{\nu_1}\Bigg(\frac{1}{2}\sum_{\nu_2}[{}^{(1)}_{3}G_V]_{\nu_1,\nu_2,\nu_2}\,\bar{\omega}_{\nu_2} + \frac{1}{2}[{}^{(1)}_{1}G_V]_{\nu_1}\bar{\omega}_{\nu_1}$$
$$+[{}^{(1)}_{1}F_V]_{\nu_1}\Bigg)q'_{\nu_1}. \tag{38}$$

We define the $(4\times4\times4)$ tensor $\tau^{H_1}_{\mu_1,\mu_2,\mu_3}$ and the length-4 column vector $\tau^{H_1}_{\mu_1}$ so that the above equation may be written in terms of Clebsch-Gordan coefficients of S_N, $C^{\mu_1\mu_2\mu_3\mathcal{R}}_{\xi_1,\xi_2,\xi_3}$ (see Sec. V.B in Ref. [25]), and their coefficient tensors

$$\tau^{H_1}_{\mu_1,\mu_2,\mu_3,\mathcal{R}} = -\frac{1}{2}\,{}^{(1)}_{3}\tau^{G}_{\mu_1,\mu_2,\mu_3,\mathcal{R}}\,\bar{\omega}_{\mu_2}\bar{\omega}_{\mu_3} + \frac{1}{3!}\,{}^{(1)}_{3}\tau^{F}_{\mu_1,\mu_2,\mu_3,\mathcal{R}}, \tag{39}$$

$$\tau^{H_1}_{\mu_1} = \frac{1}{2}\sum_{\mu_2} d_{\mu_2}\, {}^{(1)}_{3}\tau^{G}_{\mu_1,\mu_2,\mu_2,I}\bar{\omega}_{\mu_2} + \frac{1}{2}\, {}^{(1)}_{1}\tau^{G}_{\mu_1}\bar{\omega}_{\mu_1} + {}^{(1)}_{1}\tau^{F}_{\mu_1}, \tag{40}$$

where repeated μ_2 and μ_3 indices in Eq. (39) and repeated μ_1 indices in Eq. (40) are not summed over. Therefore, the polynomial $(\bar{H}_1)_{\text{eff}}$ may be written in the following compact form:

$$\begin{aligned}(\bar{H}_1)_{\text{eff}} = &\sum_{\mu_1,\mu_2,\mu_3,\mathcal{R}} \tau^{H_1}_{\mu_1,\mu_2,\mu_3,\mathcal{R}} \\ &\times \sum_{\xi_1,\xi_2,\xi_3} C^{\mu_1\mu_2\mu_3\mathcal{R}}_{\xi_1,\xi_2,\xi_3}\,[q'_{\mu_1}]_{\xi_1}\,[q'_{\mu_2}]_{\xi_2}\,[q'_{\mu_3}]_{\xi_3} \\ &+ \sum_{\mu=\{\mathbf{0}+,\mathbf{0}-\}} \tau^{H_1}_{\mu} q'_{\mu}.\end{aligned} \tag{41}$$

2. Derivation of the cubic Δ

From Eqs. (32) and (41) (in Sec. II G 1), we obtain the polynomial equation

$$[\Delta, H_0]\Phi_0 = (\bar{H}_1)_{\text{eff}}\,\Phi_0. \tag{42}$$

Solving this equation for the polynomial Δ, we obtain

$$\begin{aligned}\Delta = &\sum_{\mu_1,\mu_2,\mu_3,\mathcal{R}} \sum_{\xi_1,\xi_2,\xi_3} ({}^{(1)}_{3}\tau^{\Delta}_{\mu_1,\mu_2,\mu_3,\mathcal{R}}\, C^{\mu_1\mu_2\mu_3,\mathcal{R}}_{\xi_1,\xi_2,\xi_3}) \\ &\times [q'_{\mu_1}]_{\xi_1}[q'_{\mu_2}]_{\xi_2}[q'_{\mu_3}]_{\xi_3} + \sum_{\mu=\{\mathbf{0}+,\mathbf{0}-\}} {}^{(1)}_{1}\tau^{\Delta}_{\mu}\, q'_{\mu},\end{aligned} \tag{43}$$

where

$${}^{(1)}_{3}\tau^{\Delta}_{\mu_1,\mu_2,\mu_3,R} = \frac{-\,{}^{(1)}_{3}\tau^{H_1}_{\mu_1,\mu_2,\mu_3,R}}{\bar{\omega}_{\mu_1} + \bar{\omega}_{\mu_2} + \bar{\omega}_{\mu_3}}, \tag{44}$$

$${}^{(1)}_{1}\tau^{\Delta}_{\mathbf{0}^{\pm}} = \frac{1}{\bar{\omega}_{\mathbf{0}^{\pm}}}[-\,{}^{(1)}_{1}\tau^{H_1}_{\mathbf{0}^{\pm}} \tag{45}$$

$$+ \sum_{\mu} d_{\mu}({}^{(1)}_{3}\tau^{\Delta}_{\mathbf{0}^{\pm}\mu\mu} + {}^{(1)}_{3}\tau^{\Delta}_{\mu\mathbf{0}^{\pm}\mu} + {}^{(1)}_{3}\tau^{\Delta}_{\mu\mu\mathbf{0}^{\pm}})]. \tag{46}$$

Therefore, the first-order many body wave function is obtained by multiplying the lowest-order wave function by Δ, a polynomial in $\mathbf{q}'$ given by Eqs. (43) and (44),

$$\Phi_1(\mathbf{q}') = (1 + \delta^{1/2}\Delta)\Phi_0(\mathbf{q}'). \tag{47}$$

III. DERIVATION OF THE DENSITY PROFILE FOR THE WAVE FUNCTION THROUGH FIRST ORDER

A. Recap: The lowest-order density profile

In Ref. [23], we derived the Jacobian-weighted density profile at lowest order by integrating over many of the degrees of freedom of the wave function and transforming that integral from normal to internal coordinates. We arrived at (Eq. (68) in Ref. [23])

$$S(D)\mathcal{N}_0(r) = N\sqrt{\frac{D}{\kappa^2(D)}\frac{R}{\pi}}\exp\left[-R\left(r\frac{\sqrt{D}}{\kappa(D)} - \sqrt{D}\bar{r}_{\infty}\right)^2\right]. \tag{48}$$

The factor $S(D)$ is the D-dimensional solid angle [27],

$$S(D) = \frac{2\pi^{D/2}}{\Gamma\left(\frac{D}{2}\right)}, \tag{49}$$

and the quantity R (a number) is defined in Eq. (87) below.

Notice that the lowest-order Jacobian-weighted density profile is a Gaussian (normalized to N) centered around $r = \kappa(D)\bar{r}_{\infty}$, the $D\to\infty$ configuration radius in oscillator units (see Eqs. (9) and (13) in Ref. [23]). The form of this Gaussian function is flexible in the sense that its shape depends on the values of two quantities, R and $\bar{r}_{\infty}$. However, this lowest-order Jacobian-weighted density profile is still limited to a symmetric shape about $r=\kappa(D)\bar{r}_{\infty}$. The corrections derived from the first-order wave function will add further flexibility by allowing for asymmetry.

B. Density profile corrections from the wave function through first order

The derivation of the density profile for the first-order wave function is similar to that of the lowest-order density profile in that the same transformations are used to perform a change of coordinates. Integrals over the normal coordinates $\boldsymbol{q}'_{\mathbf{0}^+}$, $\boldsymbol{q}'_{\mathbf{0}^-}$, $[\boldsymbol{q}'_{\mathbf{1}^+}]_{N-1}$, and $[\boldsymbol{q}'_{\mathbf{1}^-}]_{N-1}$ are transformed to $\bar{r}'_N$, $\bar{r}'_S$, $\boldsymbol{S}^{[N]}_{\bar{\boldsymbol{\gamma}}'}$, and $[\boldsymbol{S}^{[N-1,1]}_{\bar{\boldsymbol{\gamma}}'}]_{(N-1)}$, where

$$\bar{r}'_S = \sum_{i=1}^{N-1} \bar{r}'_i. \tag{50}$$

The density profile for the first-order wave function is derived from the first-order wave function in a similar way the to lowest-order derivation. In Ref. [23] we showed that we can write

$$\begin{aligned}S(D)\mathcal{N}(r) = N\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\delta_f(r - r_N) \\ \times\left[{}_{g}[\Phi(\bar{\mathbf{y}}')]^2 \prod_{\mu=\mathbf{0}^{\pm},\mathbf{1}^{\pm},\mathbf{2}}\prod_{\xi=1}^{d_\mu} d[q'_{\mu}]_{\xi}\right].\end{aligned} \tag{51}$$

By simply substituting $[{}_{g}\Phi_1(\bar{\mathbf{q}}')]^2 = L_1^2(1+\delta^{1/2}\Delta)^2[{}_{g}\Phi_0(\bar{\mathbf{q}}')]^2$ for $[{}_{g}\Phi(\bar{\mathbf{q}}')]^2$ in Eq. (51), where L_1 is the normalization constant for the wave function through first order, we obtain the density profile for the first-order wave function as

$$\begin{aligned}\mathcal{N}_1(r) = &\frac{NL_1^2}{S(D)}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\prod_{\mu=\mathbf{0}^{\pm},\mathbf{1}^{\pm},\mathbf{2}}\prod_{\xi=1}^{d_\mu} d[q'^{\mu}]_{\xi} \\ &\times \delta_f(r - r_N)(1 + 2\delta^{1/2}\Delta + \delta\Delta^2)[{}_{g}\Phi_0(\bar{\mathbf{q}}')]^2 \\ = &L_1^2[1 + \delta^{1/2}\,{}_{1}\mathcal{N}_1(r) + \delta\,{}_{2}\mathcal{N}_1(r)]\mathcal{N}_0(r),\end{aligned} \tag{52}$$

where $\delta_f(r-r_i)$ is the Dirac delta function (differentiated from the inverse dimension, δ, by the subscript f). Since the

density profile is a positive quantity (it involves the square of the wave function, a real quantity), for $\mathcal{N}_1(r)$ to be a positive function of r for all real positive δ implies a relationship between ${}_1\mathcal{N}_1(r)$ and ${}_2\mathcal{N}_1(r)$, specifically

$$ {}_2\mathcal{N}_1(r) = \frac{[{}_1\mathcal{N}_1(r)]^2}{4}, \tag{53}$$

so that

$$ \mathcal{N}_1(r) = L_1^2\left[1 + \delta^{1/2}\frac{{}_1\mathcal{N}_1(r)}{2}\right]^2 \mathcal{N}_0(r). \tag{54}$$

Thus to derive the density profile, $\mathcal{N}_1(r)$, from the through first-order wave function we only have to derive ${}_1\mathcal{N}_1(r)$ [L_1 and ${}_2\mathcal{N}_1(r)$ are determined by ${}_1\mathcal{N}_1(r)$ through Eq. (53)].

From Eq. (54), the correction to first order in $\delta^{1/2}$ to the lowest-order Jacobian-weighted density profile is

$$\begin{aligned}
&\delta^{1/2}L_1^2\ {}_1\mathcal{N}_1(r)\mathcal{N}_0(r) \\
&= \frac{NL_1^2}{S(D)}2\delta^{1/2}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\prod_{\mu=\mathbf{0}^{\pm},\mathbf{1}^{\pm},\mathbf{2}}\prod_{\xi=1}^{d_\mu} d[q'_\mu]_\xi \\
&\times \delta_f(r-r_N)\Delta[{}_g\Phi_0(\bar{\mathbf{q}}')]^2.
\end{aligned} \tag{55}$$

Substituting Δ from Eq. (43), we obtain

$$\begin{aligned}
&{}_1\mathcal{N}_1(r)\mathcal{N}_0(r) \\
&= \frac{N}{S(D)}2\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\prod_{\mu=\mathbf{0}^{\pm},\mathbf{1}^{\pm},\mathbf{2}}\prod_{\xi=1}^{d_\mu} d[q'_\mu]_\xi\ \delta_f(r-r_N) \\
&\times\left(\sum_{\mu_1,\mu_2,\mu_3,\mathcal{R}}\sum_{\xi_1,\xi_2,\xi_3} {}_3^{(1)}\tau^{\Delta}_{\mu_1,\mu_2,\mu_3,\mathcal{R}}\right. \\
&\left.\times C^{\mu_1\mu_2\mu_3,\mathcal{R}}_{\xi_1,\xi_2,\xi_3}[q'_{\mu_1}]_{\xi_1}[q'_{\mu_2}]_{\xi_2}[q'_{\mu_3}]_{\xi_3} + \sum_{\mu=\{\mathbf{0}+,\mathbf{0}-\}} {}_1^{(1)}\tau^{\Delta}_{\mu}\, q'_\mu\right) \\
&\times[{}_g\Phi_0(\bar{\mathbf{q}}')]^2,
\end{aligned} \tag{56}$$

where μ_1, μ_2, and μ_3 each run over $\mathbf{0}^+$, $\mathbf{0}^-$, $\mathbf{1}^+$ $\mathbf{1}^-$, and $\mathbf{2}$, and $1\le\xi_1,\xi_2,\xi_3\le d_\mu$ where $d_\mu=1$, $N-1$, and $N(N-3)/2$ for $\mu=\mathbf{0}^{\pm}$, $\mathbf{1}^{\pm}$, and $\mathbf{2}$, respectively. When $\mu=\mathbf{2}$, $I\le\mathcal{R}\le II$; otherwise $\mathcal{R}=I$.

1. Normal coordinate integrals

We simplify Eq. (56) by defining the $(P\times P\times P)$ tensor ${}_3M_{\nu_1,\nu_2,\nu_3}$ of integrals and the length P column vector ${}_1M_\nu$ of integrals as special cases of the rank n tensor of integrals,

$$\begin{aligned}
{}_nM_{\nu_1,\nu_2,\ldots,\nu_n} &= \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\prod_{\mu=\mathbf{0}^{\pm},\mathbf{1}^{\pm},\mathbf{2}}\prod_{\xi=1}^{d_\mu} d[q'_\mu]_\xi\ \delta_f(r-r_N) \\
&\times q'_{\nu_1}q'_{\nu_2}\cdots q'_{\nu_n}[{}_g\Phi_0(\bar{\mathbf{q}}')]^2.
\end{aligned} \tag{57}$$

Indexing ${}_3M$ and ${}_1M$ by (μ_i,ξ_i) rather than ν_i (see Table III of Ref. [29]), we can write the density profile as a tensor contraction,

$$ {}_1\mathcal{N}_1(r)\mathcal{N}_0(r) = \frac{2N}{S(D)}\left(\sum_{\mu_1,\mu_2,\mu_3,\mathcal{R}}\sum_{\xi_1,\xi_2,\xi_3} {}_3^{(1)}\tau^{\Delta}_{\mu_1,\mu_2,\mu_3,\mathcal{R}}\, C^{\mu_1\mu_2\mu_3,\mathcal{R}}_{\xi_1,\xi_2,\xi_3}\, {}_3M^{\mu_1\mu_2\mu_3}_{\xi_1,\xi_2,\xi_3} + \sum_{\mu=\{\mathbf{0}+,\mathbf{0}-\}} {}_1^{(1)}\tau^{\Delta}_{\mu}\, {}_1M^{\mu}_1\right). \tag{58}$$

Each element of the M tensor is an integral.

Due to the presence of the Dirac delta function in ${}_3M$ and ${}_1M$ we must treat integrals over normal coordinates involving r_N differently from those that do not involve r_N. As in Ref. [23] which derives the lowest-order density profile $\mathcal{N}_0(r)$, we note that r_N appears in only four normal coordinates, i.e., in $\boldsymbol{q}'_{\mathbf{0}^+}$, $\boldsymbol{q}'_{\mathbf{0}^-}$, $[\boldsymbol{q}'_{\mathbf{1}^+}]_{d_{\mathbf{1}^+}}$, and $[\boldsymbol{q}'_{\mathbf{1}^-}]_{d_{\mathbf{1}^-}}$ [see Eqs. (26)–(28)]. The remaining $[N(N+1)/2-4]$ integrals, the overwhelming majority of the integrals, are easily evaluated using the integral identity

$$\int_{-\infty}^{\infty}\sqrt{\frac{\bar{\omega}_\nu}{\pi}}(q'_\nu)^m e^{-\bar{\omega}_\nu(q'_\nu)^2}dq'_\nu = \frac{[1+\exp(im\pi)]}{2\sqrt{\pi}\bar{\omega}_\nu^{m/2}}\Gamma\left(\frac{m+1}{2}\right), \tag{59}$$

which is zero when m is odd. Thus many terms are zeroed out; only those terms involving even powers of the normal coordinates which are independent of r_N contribute.

Thus from Eqs. (58) and (59) we find

$$\begin{aligned}
{}_1\mathcal{N}_1(r)\mathcal{N}_0(r) = \frac{2N}{S(D)}\Bigg\{&\sum_{\mu'_1,\mu'_2,\mu'_3} {}_3^{(1)}\tau^{\Delta}_{\mu'_1,\mu'_2,\mu'_3,I}\, C^{\mu'_1\mu'_2\mu'_3,I}_{d_{\mu'_1},d_{\mu'_2},d_{\mu'_3}}\, {}_3M^{\mu'_1\mu'_2\mu'_3}_{d_{\mu'_1},d_{\mu'_2},d_{\mu'_3}} \\
&+\sum_{\mu'}\left[\sum_{\bar{\mu}}\frac{1}{2\bar{\omega}_{\bar{\mu}}}({}_3^{(1)}\tau^{\Delta}_{\bar{\mu},\bar{\mu},\mu',I}+{}_3^{(1)}\tau^{\Delta}_{\bar{\mu},\mu',\bar{\mu},I}+{}_3^{(1)}\tau^{\Delta}_{\mu',\bar{\mu},\bar{\mu},I})C^{\bar{\mu}\bar{\mu}\mu',I}_{\bar{\xi},\bar{\xi},d_{\mu'}} + \delta_{\mu',\mathbf{0}^{\pm}}\,{}_1^{(1)}\tau^{\Delta}_{\mu'}\right]{}_1M^{\mu'}_{d_{\mu'}}\Bigg\},
\end{aligned} \tag{60}$$

where all primed indices range over $\mathbf{0}^{\pm}$ and $\mathbf{1}^{\pm}$, $\delta_{\mu',\mathbf{0}^{\pm}}$ equals 1 when $\mu'=\mathbf{0}^{\pm}$ but is 0 otherwise, $\bar{\mu}$ ranges over $\mathbf{1}^{\pm}$ and $\mathbf{2}$, and $1\leq\bar{\xi}\leq d_{\mathbf{1}^{\pm}}-1=N-2$ when $\bar{\mu}=\mathbf{1}^{\pm}$ or $1\leq\bar{\xi}\leq d_{\mathbf{2}}=N(N-3)/2$ when $\bar{\mu}=\mathbf{2}$.

2. Clebsch-Gordan tensor contractions

The relevant Clebsch-Gordan elements and sums in the above equation are

$$C_{1\ 1\ 1}^{\mathbf{0}\ \mathbf{0}\ \mathbf{0},I}=1,$$

$$C_{N-1\ 1\ 1}^{\mathbf{1}\ \mathbf{0}\ \mathbf{0},I}=C_{1\ N-1\ 1}^{\mathbf{0}\ \mathbf{1}\ \mathbf{0},I}=C_{1\ 1\ N-1}^{\mathbf{0}\ \mathbf{0}\ \mathbf{1},I}=0,$$

$$C_{N-1\ N-1\ 1}^{\mathbf{1}\ \mathbf{1}\ \mathbf{0},I}=C_{N-1\ 1\ N-1}^{\mathbf{1}\ \mathbf{0}\ \mathbf{1},I}=C_{1\ N-1\ N-1}^{\mathbf{0}\ \mathbf{1}\ \mathbf{1},I}=1, \tag{61}$$

$$C_{N-1\ N-1\ N-1}^{\mathbf{1}\ \mathbf{1}\ \mathbf{1},I}=\frac{-(N-2)}{\sqrt{N(N-1)}},$$

$$\sum_{\bar{\xi}=1}^{N-2} C_{\bar{\xi}\ \bar{\xi}\ 1}^{\mathbf{1}\ \mathbf{1}\ \mathbf{0},I}=N-2, \tag{62}$$

$$\sum_{\bar{\xi}=1}^{N(N-3)/2} C_{\bar{\xi}\ \bar{\xi}\ 1}^{\mathbf{2}\ \mathbf{2}\ \mathbf{0},I}=\frac{N(N-3)}{2}, \tag{63}$$

$$\sum_{\bar{\xi}=1}^{N-2} C_{\bar{\xi}\ \bar{\xi}\ N-1}^{\mathbf{1}\ \mathbf{1}\ \mathbf{1},I}=\frac{N-2}{\sqrt{N(N-1)}}, \tag{64}$$

$$\sum_{\bar{\xi}=1}^{N(N-3)/2} C_{\bar{\xi}\ \bar{\xi}\ N-1}^{\mathbf{2}\ \mathbf{2}\ \mathbf{1},I}=0. \tag{65}$$

Equation (65) simply follows from the fact that since the **2** irrep. indices are saturated, there is nothing to couple the **1** irrep. index with to form a scalar **0** irrep.

Equation (60) may be further simplified by defining two tensors which hold the coefficients of the elements of ${}_3M_{d_{\mu_1'},d_{\mu_2'},d_{\mu_3'}}^{\mu_1'\mu_2'\mu_3'}$ and ${}_1M_{d_{\mu'}}^{\mu'}$ tensors. We define a $4\times4\times4$ tensor, ${}^3E_{\mu_1',\mu_2',\mu_3'}$, to be the nonzero coefficients of the elements of ${}_3M_{d_{\mu_1'},d_{\mu_2'},d_{\mu_3'}}^{\mu_1'\mu_2'\mu_3'}$ (which are cubic in r_N),

$${}^3E_{\mu_1',\mu_2',\mu_3'}={}_3^{(1)}\tau_{\mu_1',\mu_2',\mu_3',I}^{\Delta}\,C_{d_{\mu_1'},d_{\mu_2'},d_{\mu_3'}}^{\mu_1'\mu_2'\mu_3',I}. \tag{66}$$

We emphasize that the above equation is a simple elemental multiplication; no summation is implied. Using the above Clebsch-Gordan elements, we obtain

$${}^3E_{\mathbf{0}^{\pm},\mathbf{0}^{\pm},\mathbf{0}^{\pm}}=\tau_{\mathbf{0}^{\pm},\mathbf{0}^{\pm},\mathbf{0}^{\pm}}^{\Delta}, \tag{67}$$

$${}^3E_{\mathbf{1}^{\pm},\mathbf{0}^{\pm},\mathbf{0}^{\pm}}={}^3E_{\mathbf{0}^{\pm},\mathbf{1}^{\pm},\mathbf{0}^{\pm}}={}^3E_{\mathbf{0}^{\pm},\mathbf{0}^{\pm},\mathbf{1}^{\pm}}=0, \tag{68}$$

$${}^3E_{\mathbf{1}^{\pm},\mathbf{1}^{\pm},\mathbf{0}^{\pm}}=\tau_{\mathbf{1}^{\pm},\mathbf{1}^{\pm},\mathbf{0}^{\pm}}^{\Delta}, \tag{69}$$

$${}^3E_{\mathbf{0}^{\pm},\mathbf{0}^{\pm},\mathbf{1}^{\pm}}=\tau_{\mathbf{1}^{\pm},\mathbf{0}^{\pm},\mathbf{0}^{\pm}}^{\Delta}, \tag{70}$$

$${}^3E_{\mathbf{0}^{\pm},\mathbf{1}^{\pm},\mathbf{1}^{\pm}}=\tau_{\mathbf{0}^{\pm},\mathbf{1}^{\pm},\mathbf{1}^{\pm}}^{\Delta}, \tag{71}$$

$${}^3E_{\mathbf{1}^{\pm},\mathbf{1}^{\pm},\mathbf{1}^{\pm}}=\frac{-(N-2)}{\sqrt{N(N-1)}}\tau_{\mathbf{1}^{\pm},\mathbf{1}^{\pm},\mathbf{1}^{\pm}}^{\Delta}. \tag{72}$$

In Eqs. (67)–(72), each $\pm$ associated with a sector μ is taken to be independent of the $\pm$ associated with the other two sectors.

We also define a length-four column vector ${}^1E_{\mu'}$ to be the nonzero coefficients of the elements of ${}_1M_{d_{\mu'}}^{\mu'}$ (which are linear in r_N),

$${}^1E_{\mu'}=\sum_{\bar{\mu}}\frac{1}{2\bar{\omega}_{\bar{\mu}}}({}_3^{(1)}\tau_{\bar{\mu},\bar{\mu},\mu',I}^{\Delta}+{}_3^{(1)}\tau_{\bar{\mu},\mu',\bar{\mu},I}^{\Delta}+{}_3^{(1)}\tau_{\mu',\bar{\mu},\bar{\mu},I}^{\Delta})\sum_{\bar{\xi}}C_{\bar{\xi},\bar{\xi},d_{\mu'}}^{\bar{\mu}\bar{\mu}\mu',I}+\delta_{\mu',\mathbf{0}^{\pm}}\,{}_1^{(1)}\tau_{\mu'}^{\Delta}, \tag{73}$$

i.e.,

$$\begin{aligned}{}^1E_{\mathbf{0}^{\pm}}=&\frac{(N-2)}{2}\frac{1}{\omega_{\mathbf{1}^+}}(\tau_{\mathbf{1}^+\mathbf{1}^+\mathbf{0}^{\pm}}^{\Delta}+\tau_{\mathbf{1}^+\mathbf{0}^{\pm}\mathbf{1}^+}^{\Delta}+\tau_{\mathbf{0}^{\pm}\mathbf{1}^+\mathbf{1}^+}^{\Delta})\\&+\frac{(N-2)}{2}\frac{1}{\omega_{\mathbf{1}^-}}(\tau_{\mathbf{1}^-\mathbf{1}^-\mathbf{0}^{\pm}}^{\Delta}+\tau_{\mathbf{1}^-\mathbf{0}^{\pm}\mathbf{1}^-}^{\Delta}+\tau_{\mathbf{0}^{\pm}\mathbf{1}^-\mathbf{1}^-}^{\Delta})\\&+\frac{N(N-3)}{4}\frac{1}{\omega_{\mathbf{2}}}(\tau_{\mathbf{220}^{\pm}}^{\Delta}+\tau_{\mathbf{20}^{\pm}\mathbf{2}}^{\Delta}+\tau_{\mathbf{0}^{\pm}\mathbf{22}}^{\Delta})+{}_1^{(1)}\tau_{\mathbf{0}^{\pm}}^{\Delta},\end{aligned} \tag{74}$$

$$\begin{aligned}{}^1E_{\mathbf{1}^{\pm}}=&\frac{N-2}{2\sqrt{N(N-1)}}\frac{1}{\omega_{\mathbf{1}^+}}({}_3^{(1)}\tau_{\mathbf{1}^+\mathbf{1}^+\mathbf{1}^{\pm}}^{\Delta}+{}_3^{(1)}\tau_{\mathbf{1}^+\mathbf{1}^{\pm}\mathbf{1}^+}^{\Delta}+{}_3^{(1)}\tau_{\mathbf{1}^{\pm}\mathbf{1}^+\mathbf{1}^+}^{\Delta})\\&+\frac{N-2}{2\sqrt{N(N-1)}}\frac{1}{\omega_{\mathbf{1}^-}}({}_3^{(1)}\tau_{\mathbf{1}^-\mathbf{1}^-\mathbf{1}^{\pm}}^{\Delta}+{}_3^{(1)}\tau_{\mathbf{1}^-\mathbf{1}^{\pm}\mathbf{1}^-}^{\Delta}+{}_3^{(1)}\tau_{\mathbf{1}^{\pm}\mathbf{1}^-\mathbf{1}^-}^{\Delta}).\end{aligned} \tag{75}$$

Using Eqs. (66) and (73), Eq. (60) may be written in a simpler form as

$${}_1\mathcal{N}_1(r)\mathcal{N}_0(r)=\frac{2N}{S(D)}\left(\sum_{\mu_1',\mu_2',\mu_3'}{}^3E_{\mu_1',\mu_2',\mu_3'}\,{}_3M_{d_{\mu_1'},d_{\mu_2'},d_{\mu_3'}}^{\mu_1'\mu_2'\mu_3'}+\sum_{\mu'}{}^1E_{\mu'}\,{}_1M_{d_{\mu'}}^{\mu'}\right). \tag{76}$$

3. Transformation of the integrals to symmetry coordinates

The elements of the M tensors are integrals over the normal coordinates. We use the $\boldsymbol{T}$ transformation in Ref. [23], where

$$\begin{pmatrix} \boldsymbol{q}'^{\mathbf{0}^+} \\ \boldsymbol{q}'^{\mathbf{0}^-} \\ [\boldsymbol{q}'^{\mathbf{1}^+}]_{N-1} \\ [\boldsymbol{q}'^{\mathbf{1}^-}]_{N-1} \end{pmatrix} = \boldsymbol{T}\boldsymbol{a}', \tag{77}$$

to write these M tensors in terms of integrals over the coordinates of the four-element vector

$$\boldsymbol{a}' = \begin{pmatrix} \bar{r}'_N \\ \boldsymbol{b}' \end{pmatrix}, \tag{78}$$

where

$$\boldsymbol{b}' = \begin{pmatrix} \bar{r}'_S \\ \boldsymbol{S}^{[N]}_{\bar{\gamma}'} \\ [\boldsymbol{S}^{[N-1,1]}_{\bar{\gamma}'}]_{(N-1)} \end{pmatrix}, \tag{79}$$

i.e.,

$${}_nM^{\mu'_1\mu'_2\ldots\mu'_n}_{d_{\mu'_1}d_{\mu'_2}\ldots d_{\mu'_n}} = \sum_{i_1,i_2,\ldots,i_n} T_{\mu'_1,i_1}T_{\mu'_2,i_2}\ldots T_{\mu'_n,i_n}\ {}_n\mathcal{M}_{i_1i_2\ldots i_n}, \tag{80}$$

where $\boldsymbol{T}$ is given in Eqs. (53)–(55) in Ref. [23]. Applying the analysis of Sec. VIII in Ref. [23] to the ${}_n\mathcal{M}_{i_1i_2\ldots i_n}$ tensor, we arrive at

$$\begin{aligned} {}_n\mathcal{M}_{i_1i_2\ldots i_n} = {} & \frac{J_T\sqrt{\bar{\omega}_{\mathbf{0}^+}\bar{\omega}_{\mathbf{0}^-}\bar{\omega}_{\mathbf{1}^+}\bar{\omega}_{\mathbf{1}^-}}}{\pi^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\delta_f(r-a_1) \\ & \times a_{i_1}a_{i_2}\ldots a_{i_n}\exp(-K_0a_1^2 - 2a_1\boldsymbol{K}^T\boldsymbol{b}' \\ & - \boldsymbol{b}'^T\boldsymbol{\mathcal{K}}\boldsymbol{b}')\,da_1\,d^3\boldsymbol{b}', \end{aligned} \tag{81}$$

where K_0, $\boldsymbol{K}$, and $\boldsymbol{\mathcal{K}}$ are defined in Eqs. (59)–(61), respectively, in Ref. [23] and J_T is the Jacobian of the transformation from $\boldsymbol{q}'_{\mathbf{0}^+}$, $\boldsymbol{q}'_{\mathbf{0}^-}$, $[\boldsymbol{q}'_{\mathbf{1}^+}]_{d_{\mathbf{1}^+}}$, and $[\boldsymbol{q}'_{\mathbf{1}^-}]_{d_{\mathbf{1}^-}}$ to the internal coordinates $\boldsymbol{a}'$ (Eq. (55) in Ref. [23]).

Substituting Eq. (80) into Eq. (76) we obtain the density profile in terms of integrals over internal coordinates, i.e.,

$${}_1\mathcal{N}_1(r)\mathcal{N}_0(r) = \frac{2N}{S(D)}\left(\sum_{i_1,i_2,i_3} {}_3\Xi_{i_1i_2i_3}\ {}_3\mathcal{M}_{i_1i_2i_3} + \sum_i {}_1\Xi_i\ {}_1\mathcal{M}_i\right), \tag{82}$$

where the (length 4) column vector ${}_1\Xi_i$ and the $(4\times4\times4)$ tensor ${}_3\Xi_{i,j,k}$ are

$${}_1\Xi_i = \sum_{\mu'} {}^1E_{\mu'}T_{\mu',i}, \tag{83}$$

$${}_3\Xi_{i_1i_2i_3} = \sum_{\mu'_1,\mu'_2,\mu'_3} {}^3E_{\mu'_1,\mu'_2,\mu'_3}\,T_{\mu'_1,i_1}\,T_{\mu'_2,i_2}\,T_{\mu'_3,i_3}. \tag{84}$$

4. Evaluation of the integrals

To perform the integrals of Eq. (81) for ${}_3\mathcal{M}_{i_1i_2i_3}$ and ${}_1\mathcal{M}_i$ in Eq. (82), we define the four-component vector

$$\boldsymbol{V} = \begin{pmatrix} \frac{1}{2}K_0 \\ \boldsymbol{K} \end{pmatrix}. \tag{85}$$

Equation (81) can be written as a series of derivatives of a term proportional to $\mathcal{N}_0(r)$,

$$\begin{aligned} {}_n\mathcal{M}_{i_1i_2\ldots i_n} = {} & \frac{\sqrt{\det\boldsymbol{\mathcal{K}}}R}{\pi^2}\times\left(\frac{-1}{2\bar{r}'}\frac{\partial}{\partial V_{i_1}}\right) \\ & \times\left(\frac{-1}{2\bar{r}'}\frac{\partial}{\partial V_{i_2}}\right)\ldots\left(\frac{-1}{2\bar{r}'}\frac{\partial}{\partial V_{i_n}}\right) \\ & \times\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\delta_f(r-a_1) \\ & \times\exp(-K_0\,a_1^2 - 2a_1\boldsymbol{K}^T\boldsymbol{b}' - \boldsymbol{b}'^T\boldsymbol{\mathcal{K}}\boldsymbol{b}')\,da_1d^3\boldsymbol{b}', \end{aligned} \tag{86}$$

where we have also used Eq. (67) in Ref. [23],

$$R = \frac{\bar{\omega}_{\mathbf{0}^+}\bar{\omega}_{\mathbf{0}^-}\bar{\omega}_{\mathbf{1}^+}\bar{\omega}_{\mathbf{1}^-}J_T^2}{\det\boldsymbol{\mathcal{K}}} = (K_0 - \boldsymbol{K}^T\boldsymbol{\mathcal{K}}^{-1}\boldsymbol{K}). \tag{87}$$

Upon using the integral identity

$$\begin{aligned} & \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\exp(-\boldsymbol{b}'^T\boldsymbol{\mathcal{K}}\boldsymbol{b}' - 2a_1\boldsymbol{K}^T\boldsymbol{b}')d^n\boldsymbol{b}' \\ & = \frac{\pi^{n/2}}{\sqrt{\det\boldsymbol{\mathcal{K}}}}\exp(a_1^2\boldsymbol{K}^T\boldsymbol{\mathcal{K}}^{-1}\boldsymbol{K}), \end{aligned} \tag{88}$$

in Eq. (86) we obtain

$${}_n\mathcal{M}_{i_1i_2\ldots i_n} = \sqrt{\frac{R}{\delta\kappa(D)^2\pi}} \tag{89}$$

$$\begin{aligned} & \times\left(\frac{-1}{2\bar{r}'}\frac{\partial}{\partial V_{i_1}}\right)\left(\frac{-1}{2\bar{r}'}\frac{\partial}{\partial V_{i_2}}\right)\ldots\left(\frac{-1}{2\bar{r}'}\frac{\partial}{\partial V_{i_n}}\right) \\ & \times\exp[-(K_0 - \boldsymbol{K}^T\boldsymbol{\mathcal{K}}^{-1}\boldsymbol{K})\bar{r}'^2], \end{aligned} \tag{90}$$

which yields

$$ {}_n\mathcal{M}_{i_1 i_2 \ldots i_n} = \sqrt{\frac{R}{\delta \kappa(D)^2 \pi}} \hat{C} ({}_1\chi_{i_1}\, {}_1\chi_{i_2} \times \cdots \times {}_1\chi_{i_n} \bar{r}'^{\,n} + {}_2\chi_{i_1 i_2}\, {}_1\chi_{i_3}\, {}_1\chi_{i_4} \times \cdots \times {}_1\chi_{i_n} \bar{r}'^{\,n-2} + {}_2\chi_{i_1 i_2}\, {}_2\chi_{i_3 i_4}\, {}_1\chi_{i_5}\, {}_1\chi_{i_6} \times \cdots $$
$$ \times {}_1\chi_{i_n} \bar{r}'^{\,n-4} + \cdots + \begin{cases} {}_2\chi_{i_1 i_2}\, {}_2\chi_{i_3 i_4} \times \cdots \times {}_2\chi_{i_{n-1} i_n} & \text{when } n \text{ is even} \\ {}_2\chi_{i_1 i_2}\, {}_2\chi_{i_3 i_4} \times \cdots \times {}_2\chi_{i_{n-2} i_{n-1}}\, {}_1\chi_{i_n} \bar{r}' & \text{when } n \text{ is odd,} \end{cases} \tag{91} $$

where the χ's are elements of

$$ {}_1\boldsymbol{\chi} = -\frac{1}{2} \boldsymbol{\nabla}_V(-R) = \begin{pmatrix} 1 \\ -\boldsymbol{\mathcal{K}}^{-1} \mathbf{K} \end{pmatrix}, \tag{92} $$

$$ {}_2\boldsymbol{\chi} = -\frac{1}{2} \boldsymbol{\nabla}_V \otimes {}_1\boldsymbol{\chi} = \frac{1}{2} \begin{pmatrix} 0 & 0 \\ 0 & \boldsymbol{\mathcal{K}}^{-1} \end{pmatrix}. \tag{93} $$

${}_1\boldsymbol{\chi}$ is four-dimensional vector and ${}_2\boldsymbol{\chi}$ is a 4×4-dimensional matrix. The $\hat{C}$ operator acts on each term in Eq. (91) to produce a sum of terms over all the distinct combinations of indices.

From Eq. (91) we can now evaluate each element of the $\mathcal{M}$ tensors,

$$ {}_1\mathcal{M}_i = \sqrt{\frac{R}{\delta\, \kappa(D)^2 \pi}}\, {}_1\chi_i \bar{r}', \tag{94} $$

$$ {}_3\mathcal{M}_{i_1 i_2 i_3} = \sqrt{\frac{R}{\delta\, \kappa(D)^2 \pi}} [{}_1\chi_{i_1}\, {}_1\chi_{i_2}\, {}_1\chi_{i_3} \bar{r}'^{\,3} + ({}_2\chi_{i_1 i_2}\, {}_1\chi_{i_3} + {}_2\chi_{i_1 i_3}\, {}_1\chi_{i_2} + {}_2\chi_{i_2 i_3}\, {}_1\chi_{i_1}) \bar{r}']. \tag{95} $$

C. Result: Density profile for the first-order wave function

1. Density profile in displacement coordinates

Using Eqs. (94), (95), and (82) in Eq. (54) yields the density profile

$$ \mathcal{N}_1(r) = \frac{N L_1^2}{S(D)} \sqrt{\frac{R}{\delta\, \kappa(D)^2 \pi}} \left(1 + \frac{\delta^{1/2}}{2} (A_1 \bar{r}' + A_3 \bar{r}'^{\,3})\right)^2 \times \exp(-R \bar{r}'^{\,2}), \tag{96} $$

where the quantities A_1 and A_3 in the polynomial are

$$ A_1 = 2 \left[\sum_i {}_1\chi_i\, {}_1\Xi_i + \sum_{i_1, i_2, i_3} ({}_2\chi_{i_1 i_2}\, {}_1\chi_{i_3} + {}_2\chi_{i_1 i_3}\, {}_1\chi_{i_2} + {}_2\chi_{i_2 i_3}\, {}_1\chi_{i_1})\, {}_3\Xi_{i_1 i_2 i_3} \right], \tag{97} $$

$$ A_3 = 2 \sum_{i_1, i_2, i_3} {}_1\chi_{i_1}\, {}_1\chi_{i_2}\, {}_1\chi_{i_3}\, {}_3\Xi_{i_1 i_2 i_3}, \tag{98} $$

where

$$ {}_1\Xi_i = \sum_{\mu = \{\mathbf{0}\pm, \mathbf{1}\pm\}} T_{\mu, i}\, {}^1E_\mu, \tag{99} $$

$$ {}_3\Xi_{i,j,k} = \sum_{\mu_1 = \{\mathbf{0}\pm, \mathbf{1}\pm\}} \sum_{\mu_2 = \{\mathbf{0}\pm, \mathbf{1}\pm\}} \sum_{\mu_3 = \{\mathbf{0}\pm, \mathbf{1}\pm\}} T_{\mu_1, i}\, T_{\mu_2, j}\, T_{\mu_3, k} \times {}^3E_{\mu_1, \mu_2, \mu_3}, \tag{100} $$

$$ {}_1\chi_i = \begin{cases} 1, & i = 1 \\ -(\boldsymbol{\mathcal{K}}^{-1} \mathbf{K})_{i-1}, & 1 < i \le 4, \end{cases} \tag{101} $$

and

$$ {}_2\chi_{i,j}\, {}_1\chi_k = \boldsymbol{\mathcal{K}}^{-1}_{i-1, j-1}\, {}_1\chi_k\, \Theta_{i-1} \Theta_{j-1} + \boldsymbol{\mathcal{K}}^{-1}_{j-1, k-1}\, {}_1\chi_i\, \Theta_{j-1} \Theta_{k-1} + \boldsymbol{\mathcal{K}}^{-1}_{k-1, i-1}\, {}_1\chi_j\, \Theta_{k-1} \Theta_{i-1}, \tag{102} $$

where

$$ \Theta_m = \begin{cases} 0 & \text{when } m \le 0 \\ 1 & \text{when } m \ge 1. \end{cases} \tag{103} $$

Since

$$ \int_{-\infty}^{+\infty} \left(1 + \frac{\delta^{1/2}}{2} (A_1 \bar{r}' + A_3 \bar{r}'^{\,3})\right)^2 \exp(-R \bar{r}'^{\,2}) d\bar{r}' = \frac{\sqrt{\pi}}{\sqrt{R}} \left(1 + \frac{\delta (4 A_1^2 R^2 + 12 A_1 A_3 R + 15 A_3^2)}{32 R^3}\right) \tag{104} $$

for $R > 0$, we conclude that

$$ L_1^2 = \frac{32 R^3}{32 R^3 + \delta (4 A_1^2 R^2 + 12 A_1 A_3 R + 15 A_3^2)}. \tag{105} $$

The density profile for the through first-order wave function has the form of a sixth-order polynomial multiplied by the lowest-order density profile. Note that the density profile is a function of the coordinate r, which is not the dimensionally scaled internal displacement coordinate $\bar{r}'(r; D)$. Thus one must make the following substitution in Eq. (96) to obtain the density profile as an explicit function of r:

$$ \bar{r}'(r; D) = \delta^{-1/2} \left(\frac{r}{\kappa(D)} - \bar{r}_\infty \right). \tag{106} $$

We have derived the N-body density profile for the wave function through first order in $\delta^{1/2}$. This density profile, $\mathcal{N}_1(r)$, of Eq. (96) includes the full interactions of N particles through first order in the perturbation series exactly and analytically. The details of the interactions at each order are folded into R, A_1, A_3, and $\bar{r}_\infty$.

2. Density profile in oscillator units

For the case of a system under harmonic confinement (such as the present trapped Hooke's law gas or a BEC in a

parabolic trap) we may choose an oscillator-unit scaling $\kappa(D)=D^2\bar{a}_{\rm ho}$, where

$$\bar{a}_{\rm ho}=\frac{1}{D^{3/2}}a_{\rm ho}. \tag{107}$$

Therefore

$$\kappa(D)=\sqrt{D}a_{\rm ho}, \tag{108}$$

$$\bar{r}'=\left(\frac{r}{a_{\rm ho}}-\sqrt{D}\bar{r}_\infty\right), \tag{109}$$

and defining

$$r_{\rm osc}=\frac{r}{a_{\rm ho}} \tag{110}$$

in oscillator units, we obtain the Jacobian-weighted density per particle,

$$\mathcal{N}_0(r_{\rm osc})\times\frac{S(D)}{N}=\sqrt{\frac{R}{\pi}}\exp[-R(r_{\rm osc}-\sqrt{D}\bar{r}_\infty)^2], \tag{111}$$

$$\mathcal{N}_1(r_{\rm osc})\times\frac{S(D)}{N}=L_1^2\left(1+\frac{\delta^{1/2}}{2}[A_1(r_{\rm osc}-\sqrt{D}\bar{r}_\infty)+A_3(r_{\rm osc}-\sqrt{D}\bar{r}_\infty)^3]\right)^2\times\mathcal{N}_0(r_{\rm osc})\times\frac{S(D)}{N}. \tag{112}$$

IV. TEST APPLICATION: HARMONICALLY INTERACTING PARTICLES UNDER HARMONIC CONFINEMENT

In this paper we have derived the Jacobian-weighted density profile for the wave function through first order as an example of an observable which may be derived from the *N*-body interacting wave function. We test this general formalism for the density profile by comparing it to the density profile of the analytically solvable system of *N* harmonically interacting particles in a harmonic-confining potential with Hamiltonian

$$H=\frac{1}{2}\left(\sum_i^N\left[-\frac{\partial^2}{\partial\boldsymbol{r}_i^2}+\omega_t^2\boldsymbol{r}_i^2\right]+\sum_{i<j}\omega_p^2\boldsymbol{r}_{i,j}^2\right). \tag{113}$$

The exact analytic density profile for this system is independently derived in the Appendix [see Eqs. (A48) and (A54)], and this is expanded through first order in $\delta^{1/2}$ to yield the exact density profile through first order [see Eq. (A70)]. This analysis shows that the density profile for any *N* or interaction strength follows a universal curve when a simple scaling is applied to the radial variable (it should be noted that this is not true of the wave function) and is given by

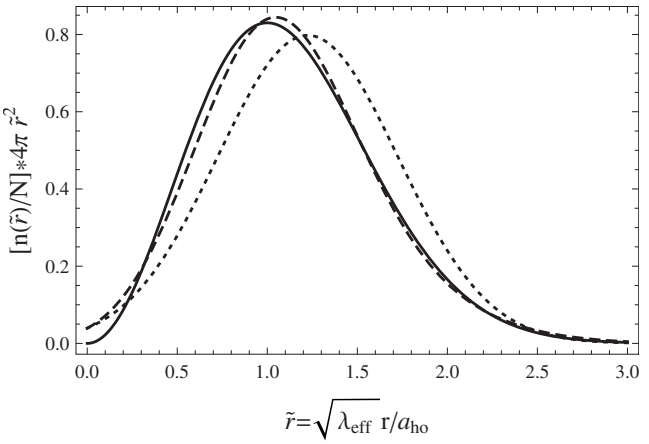

FIG. 1. Scaled density profile at $D=3$ for *N* harmonically interacting particles under harmonic confinement in oscillator units of the confining potential. The dotted curve is the lowest-order density profile, while the dashed curve is the density profile for the first-order wave function. The solid curve is the exact result. The scaling factor, $\sqrt{\lambda_{\rm eff}}$, is explained in the Appendix.

$$\mathcal{N}(\bar{r}_{\rm eff})=\frac{2D^{D/2}}{\Gamma\left(\frac{D}{2}\right)}\bar{r}_{\rm eff}^{D-1}\exp(-D\bar{r}_{\rm eff}^2), \tag{114}$$

where

$$\bar{r}_{\rm eff}=\sqrt{\lambda_{\rm eff}}\bar{r}, \tag{115}$$

$$\lambda_{\rm eff}=\frac{N\lambda}{N+\lambda-1},\quad \lambda=\sqrt{1+N\lambda_p^2},\quad \lambda_p=\omega_p/\omega_t, \tag{116}$$

and

$$\mathcal{N}(\bar{r}'_{\rm eff})=\frac{1}{\sqrt{\lambda_{\rm eff}}}\mathcal{N}(\bar{r}'). \tag{117}$$

By expanding Eq. (114) to first order and using Eq. (53) we obtain

$$\mathcal{N}_1(\bar{r}'_{\rm eff})=L_1^2\left[1+\frac{\delta^{1/2}}{2}\sqrt{2}\left(\frac{2\bar{r}'^3_{\rm eff}}{3}-\bar{r}'_{\rm eff}\right)\right]^2\left(\frac{2}{\pi}\right)^{1/2}\exp(-2\bar{r}'^2_{\rm eff}), \tag{118}$$

where

$$L_1^2=\frac{96}{96+5\delta}. \tag{119}$$

This scaled density profile for $D=3$ ($\delta=1/3$) is plotted in Fig. 1. One readily sees the improvement obtained from the first-order wave function, confirming the efficacy of this approach to the general confined *N*-body problem, which may be systematically improved by going to higher orders.

The general theory developed in this paper for the density profile involves no such harmonic interaction specific scaling since it is applicable to any interparticle potential, not just harmonic interparticle potentials. Consequently in Figs. 2 and 3 we plot the density profile for $D=3$ ($\delta=1/3$) without this harmonic-interaction specific scaling for two very differ-

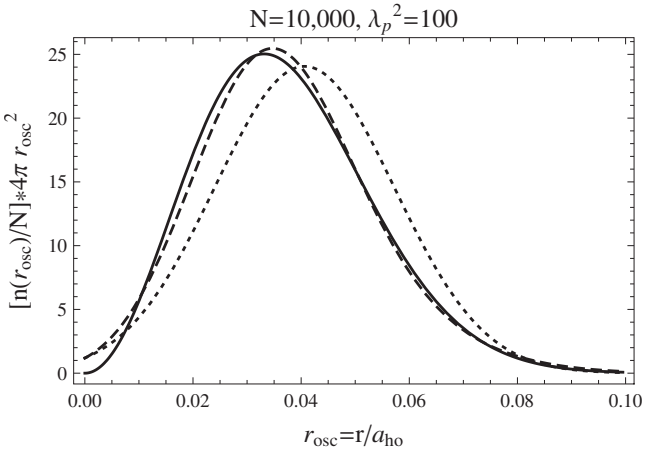

FIG. 2. Unscaled density profile at $D=3$ for $N=10\,000$ particles under harmonic confinement with strong attractive harmonic interactions ($\lambda_p^2=100$) in oscillator units of the confining potential. The dotted curve is the lowest-order density profile, while the dashed curve is the density profile for the first-order wave function. The solid curve is the exact result. The parameter λ_p^2, as explained in the Appendix, is the interaction frequency squared in oscillator units of the confining potential.

ent interparticle interaction strengths. Both are for $N=10\,000$ particles, but Fig. 2 features strongly attractive interactions, while Fig. 3 is for a repulsive interaction just below the dissociation limit. In the former case the system is tightly bound and very compact. In the latter case the confining potential is barely able to hold the system together against the combined effect of the repulsive interactions, and the system is very extended.

The density profile derived from the general N-body formalism developed in this paper and implemented in MATHEMATICA [30] code [31] is indistinguishable from the density profiles derived from the exact independent solution of the harmonically interacting system. The agreement between the general formalism, which uses a perturbation series invariant under S_N, and the direct density profiles of Eqs. (114) and (118) obtained in the Appendix, confirms the correctness of the general formalism developed in this paper and its implementation in MATHEMATICA [30] code.

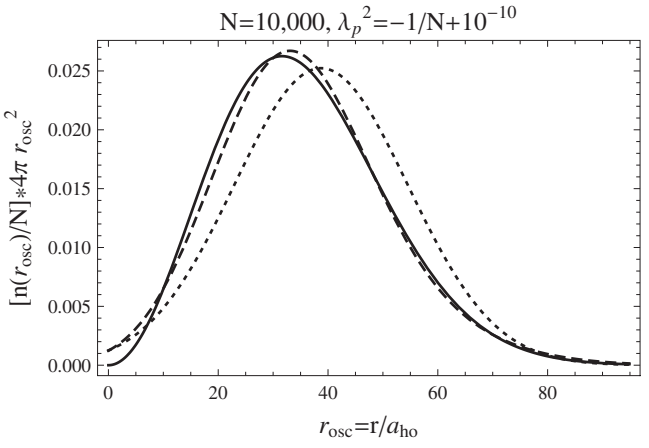

FIG. 3. Unscaled density profile at $D=3$ for $N=10\,000$ particles under harmonic confinement with repulsive harmonic interactions ($\lambda_p^2=-1/10\,000+10^{-10}$) in oscillator units of the confining potential. The system is just below the dissociation threshold and very extended. The dotted curve is the lowest-order density profile, while the dashed curve is the density profile for the first-order wave function. The solid curve is the exact result. The parameter λ_p^2, as explained in the Appendix, is the interaction frequency squared in oscillator units of the confining potential.

V. SUMMARY AND CONCLUSIONS

While the resources required to solve classical systems scale as a polynomial with the number of particles, N, allowing calculations to be performed involving large numbers of particles, the situation regarding large-N quantum systems is not so felicitous. In this case the resources required scale exponentially with N, making calculations for large-N quantum systems a far more formidable challenge unless N and the interparticle interaction strengths allow an approximation, such as the mean-field approximation.

In a series of papers, we have been developing an approach to the general interacting quantum system of N identical bosons, which while essentially analytic makes no assumptions regarding the form or strength of the interparticle interactions. This approach derives the interacting N-body wave function for identical bosons, from which any observable quantity can in principle be derived. In the process, collective normal mode coordinates are derived revealing the nature of the microscopic motions of the particles of the system for any interaction. Using this wave function, properties such as energies and density profiles have been derived.

The method involves expanding the system in inverse powers of the spatial dimension D. At large D, systems exhibit a point group structure of a far higher degree of symmetry (isomorphic to S_N) than is possible in three dimensions, allowing group theory and graphical techniques to be used to tame the exponential N scaling, leading to an essentially analytic solution at lowest order in the wave function. This large-dimension S_N point group partitions the normal modes of the system into five groups, each of which transforms under an irreducible representation of S_N. The physics of the problem involves center-of-mass excitations (for a system under harmonic confinement), breathing-mode excitations, single-particle excitations, and phonon excitations. The two normal modes which transform under scalar $[N]$ irreps. are, for a harmonic-confining potential, the center-of-mass and breathing modes; there are two groups of normal modes which transform under $[N-1,1]$ irreps. which are radial and angular single-particle modes and one group transforming under the $[N-2,2]$ irrep. for phonon modes.

More recently, in a major development of this approach, this method has been successfully extended, analytically and exactly, to first-order in the wave function, and in principle the techniques developed to do this can be extended to yet higher orders. To any finite order, the problem scales as N^0.

This paper is concerned with the application of this first-order wave function to the derivation of a physical property of interacting N-body quantum systems, namely, the density

profile of the first-order wave function. In a test of this theory, the density profile derived from the first-order wave function is tested on an exactly solvable model, namely, a system of harmonically interacting particles in a harmonic-confining potential. The harmonic interparticle interactions may be attractive or repulsive and if the interactions are sufficiently repulsive the system will dissociate despite the presence of the harmonic-confining potential.

The general theory developed in this and prior papers agrees with the exact results for this system obtained from the independent solution, showing strong convergence to the exact *three-dimensional* result for both strongly attractive interactions and repulsive interactions just below the dissociation threshold.

While this paper (as well as Ref. [19]) has focused on the harmonically interacting system in a harmonic-confining potential, the theory is not limited to these systems and in past papers we have examined other systems at lowest order, such as the Bose-Einstein condensate, *N*-electron atoms, and quantum dots. While the lowest-order approximation for the BEC captures the behavior of the system for a range of N and interaction strengths, when N or the interaction strength is larger than this range, the lowest-order density profile increasingly does not have the flexibility needed to capture the behavior of the system. The result derived from the first-order wave function does have this flexibility and so it is very desirable to apply this density profile to strongly interacting BECs as well as other strongly interacting systems. Of particular note is the fact that the functional form of the density profile of Eq. (112), derived from the first-order wave function, admits structure (wiggles) indicating the onset of crystallization or fermionization. Although such behavior is not seen for the long-range harmonic interactions examined in this paper, other systems do exhibit such transitions.

While we focused in this paper on density profiles, the theory derives the exact first-order wave function from which any observable may be derived. Also excited states may be derived, and the theory needed to extend these results to higher-angular-momentum states has been set up [32,33].

ACKNOWLEDGMENT

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APPENDIX: DENSITY PROFILE OF HARMONICALLY INTERACTING PARTICLES SUBJECT TO A HARMONIC CONFINING POTENTIAL—AN INDEPENDENT SOLUTION

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

$$H = \frac{1}{2}\left(\sum_{i}^{N}\left[-\frac{\partial^2}{\partial \boldsymbol{r}_i^2} + \omega_t^2\,\boldsymbol{r}_i^2\right] + \sum_{i<j}\omega_p^2\,\boldsymbol{r}_{i,j}^2\right). \tag{A1}$$

1. Exact *N*-body wave function

Making the orthogonal transformation to center-of-mass and Jacobi coordinates,

$$\boldsymbol{R} = \frac{1}{\sqrt{N}}\sum_{k=1}^{N}\boldsymbol{r}_k \quad \text{and} \quad \boldsymbol{\rho}_i = \frac{1}{\sqrt{i(i+1)}}\left(\sum_{j=1}^{i}\boldsymbol{r}_j - i\boldsymbol{r}_{i+1}\right), \tag{A2}$$

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

$$H = \frac{1}{2}\left(-\frac{\partial^2}{\partial \boldsymbol{R}^2} + \omega_t^2\,\boldsymbol{R}^2\right) + \frac{1}{2}\sum_{i=1}^{N-1}\left(-\frac{\partial^2}{\partial \boldsymbol{\rho}_i^2} + \omega_{\rm int}^2\,\boldsymbol{\rho}_i^2\right), \tag{A3}$$

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

$$\omega_{\rm int} = \sqrt{\omega_t^2 + N\omega_p^2}. \tag{A4}$$

The ground-state solution of the Schrödinger equation

$$H\Psi = E\Psi \tag{A5}$$

is the product of harmonic-oscillator wave functions,

$$\Psi(\boldsymbol{R},\{\boldsymbol{\rho}_i\};D) = \psi(R;\omega_t,D)\sum_{i=1}^{N-1}\psi(\rho_i;\omega_{\rm int},D), \tag{A6}$$

where $\psi(r;\omega,D)$ is the D-dimensional, harmonic-oscillator, ground-state wave function,

$$\psi(r;\omega,D) = \sqrt{\frac{\omega^{D/2}}{\pi^{D/2}}}\exp\left(-\frac{\omega}{2}r^2\right), \tag{A7}$$

and $\psi(r;\omega,D)$ satisfies the normalization condition,

$$\int_0^\infty [\psi(r;\omega,D)]^2\, r^{D-1} d^D\boldsymbol{r} = 1, \tag{A8}$$

so that

$$\int_{-\infty}^{\infty}[\Psi(\boldsymbol{R},\{\boldsymbol{\rho}_i\};D)]^2\prod_{i=1}^{N-1} d^D\boldsymbol{\rho}_i d^D\boldsymbol{R} = 1. \tag{A9}$$

2. Exact *N*-body density profile

Since the wave function is a completely symmetric function under any permutation of the particles, one can write the Jacobian-weighted density profile as

$$\mathcal{N}(r) = N\int_{-\infty}^{\infty}[\Psi(\boldsymbol{R},\{\boldsymbol{\rho}_i\};D)]^2\,\delta(r-r_N)\prod_{i=1}^{N-1} d^D\boldsymbol{\rho}_i\, d^D\boldsymbol{R}, \tag{A10}$$

where from Eqs. (A6) and (A7), the unweighted wave function is

$$\Psi(\boldsymbol{R},\{\boldsymbol{\rho}_i\};D) = \sqrt{\frac{\omega_t^{D/2}}{\pi^{D/2}}}\exp\left(-\frac{\omega_t}{2}\boldsymbol{R}^2\right)\left(\frac{\omega_{\rm int}^{D/2}}{\pi^{D/2}}\right)^{(N-1)/2} \times\prod_{i=1}^{N-1}\exp\left(-\frac{\omega_{\rm int}}{2}\boldsymbol{\rho}_i^2\right). \tag{A11}$$

Since the transformation from single-particle coordinates,

$\boldsymbol{r}_1,\ldots,\boldsymbol{r}_N$, to Jacobi and center-of-mass coordinates, $\{\boldsymbol{\rho}_i\}$ and $\boldsymbol{R}$, is orthogonal,

$$\mathcal{N}(r) = N\left(\frac{\omega_t^{D/2}}{\pi^{D/2}}\right)\left(\frac{\omega_{\rm int}^{D/2}}{\pi^{D/2}}\right)^{N-1} M(r) = r^{D-1}\rho(r), \quad \text{(A12)}$$

where $\rho(r)$ is the unweighted density profile, and

$$M(r) = \int d^D\boldsymbol{r}_1 d^D\boldsymbol{r}_2 \ldots d^D\boldsymbol{r}_N \delta(r - r_N) \times \exp[-(\omega_t - \omega_{\rm int})\boldsymbol{R}^2]\exp\left[-\omega_{\rm int}\left(\boldsymbol{R}^2 + \sum_{i=1}^{N-1}\boldsymbol{\rho}_i^2\right)\right]. \quad \text{(A13)}$$

Defining

$${}_N\boldsymbol{r} = \boldsymbol{r}_1 \oplus \boldsymbol{r}_2 \oplus \cdots \oplus \boldsymbol{r}_N = \begin{pmatrix} \boldsymbol{r}_1 \\ \boldsymbol{r}_2 \\ \vdots \\ \boldsymbol{r}_N \end{pmatrix}, \quad \text{(A14)}$$

$${}_N\boldsymbol{J} = \mathbb{J}_N \otimes \boldsymbol{I}_D, \quad \text{(A15)}$$

where $\boldsymbol{I}_D$ is the $D\times D$ dimensional unit matrix in the D-dimensional coordinate space and $\mathbb{J}_N$ is the $N\times N$ dimensional matrix of elements equal to 1 in the particle label space, then we can write

$$\boldsymbol{R}^2 = \frac{1}{N}\,{}_N\boldsymbol{r}^T\,{}_N\boldsymbol{J}\,{}_N\boldsymbol{r}, \quad \text{(A16)}$$

$$\boldsymbol{R}^2 + \sum_{i=1}^{N-1}\boldsymbol{\rho}_i^2 = \sum_{i=j}^{N}\boldsymbol{r}_j^2 = {}_N\boldsymbol{r}^T\,{}_N\boldsymbol{I}_N\boldsymbol{r}, \quad \text{(A17)}$$

where

$${}_N\boldsymbol{I} = \mathbb{I}_N \otimes \boldsymbol{I}_D, \quad \text{(A18)}$$

$\mathbb{I}_N$ is the $N\times N$ dimensional unit matrix in the particle label space. Since $\int d^D\boldsymbol{r}_N = \int r_N^{D-1} dr_N \int d\boldsymbol{\Omega}_N$, where $\int d\boldsymbol{\Omega}_N$ is the integral over the D-dimensional solid angle, we can write

$$M(r) = \int d^D\boldsymbol{r}_1 d^D\boldsymbol{r}_2 \ldots d^D\boldsymbol{r}_N \delta(r - r_N) \times \exp\left(-\frac{(\omega_t - \omega_{\rm int})}{N}\,{}_N\boldsymbol{r}^T\,{}_N\boldsymbol{J}_N\boldsymbol{r}\right)\exp(-\omega_{\rm int}\,{}_N\boldsymbol{r}^T\,{}_N\boldsymbol{I}_N\boldsymbol{r}) = S(D)r^{D-1}\exp\left(-\frac{[\omega_t + (N-1)\omega_{\rm int}]}{N}\boldsymbol{r}^2\right) \times \int d^D\boldsymbol{r}_1 d^D\boldsymbol{r}_2 \ldots d^D\boldsymbol{r}_{N-1} \times \exp(-\,{}_{N-1}\boldsymbol{r}^T\boldsymbol{A}\,{}_{N-1}\boldsymbol{r} - 2\boldsymbol{B}^T\,{}_{N-1}\boldsymbol{r}), \quad \text{(A19)}$$

where

$$S(D) = \frac{2\pi^{D/2}}{\Gamma\left(\frac{D}{2}\right)} \quad \text{(A20)}$$

is the D-dimensional solid angle,

$${}_{N-1}\boldsymbol{r} = \boldsymbol{r}_1 \oplus \boldsymbol{r}_2 \oplus \cdots \oplus \boldsymbol{r}_{N-2} \oplus \boldsymbol{r}_{N-1}, \quad \text{(A21)}$$

$$\boldsymbol{A} = \omega_{\rm int}\,{}_{N-1}\boldsymbol{I} + \frac{(\omega_t - \omega_{\rm int})}{N}\,{}_{N-1}\boldsymbol{J}, \quad \text{(A22)}$$

$$\boldsymbol{B} = \frac{(\omega_t - \omega_{\rm int})}{N}\,{}_c\boldsymbol{1}\,\boldsymbol{r}, \quad \text{(A23)}$$

$${}_{N-1}\boldsymbol{J} = \mathbb{J}_{N-1} \otimes \boldsymbol{I}_D, \quad \text{(A24)}$$

$\mathbb{J}_{N-1}$ is the $(N-1)\times(N-1)$-dimensional matrix of elements equal to 1 in the particle label space of the first $N-1$ particles,

$${}_{N-1}\boldsymbol{I} = \mathbb{I}_{N-1} \otimes \boldsymbol{I}_D, \quad \text{(A25)}$$

and $\mathbb{I}_{N-1}$ is the $(N-1)\times(N-1)$-dimensional unit matrix in the particle label space of the first $N-1$ particles,

$${}_c\boldsymbol{1} = \boldsymbol{1}_c \otimes \boldsymbol{I}_D, \quad \text{(A26)}$$

where $\boldsymbol{1}_c$ is the $(N-1)$-dimensional column vector of elements equal to 1 in the particle label space of the first $N-1$ particles so that

$${}_c\boldsymbol{1}^T\,{}_{N-1}\boldsymbol{r} = \sum_{k=1}^{N-1}\boldsymbol{r}_k. \quad \text{(A27)}$$

Using the result

$$\int_{-\infty}^{\infty} d^n\boldsymbol{b}\,\exp(-\boldsymbol{b}^T\boldsymbol{A}\boldsymbol{b} - 2\boldsymbol{B}^T\boldsymbol{b}) = \frac{\pi^{n/2}}{\sqrt{\det\boldsymbol{A}}}\exp(\boldsymbol{B}^T\boldsymbol{A}^{-1}\boldsymbol{B}) \quad \text{(A28)}$$

in Eq. (A19), with the identification $n = D(N-1)$ and $\boldsymbol{b} = \boldsymbol{r}$, we obtain

$$M(r) = S(D)\,r^{D-1}\exp\left(-\frac{[\omega_t + (N-1)\omega_{\rm int}]}{N}\boldsymbol{r}^2\right) \times \frac{\pi^{D(N-1)/2}}{\sqrt{\det\boldsymbol{A}}}\exp(\boldsymbol{B}^T\boldsymbol{A}^{-1}\boldsymbol{B}). \quad \text{(A29)}$$

Thus we need to evaluate $\det\boldsymbol{A}$ and $\boldsymbol{A}^{-1}$. First $\boldsymbol{A}^{-1}$. One has that $(\boldsymbol{U}\otimes\boldsymbol{V})^{-1} = \boldsymbol{U}^{-1}\otimes\boldsymbol{V}^{-1}$. Thus writing

$$\boldsymbol{U} = \alpha\mathbb{I}_{N-1} + \beta\mathbb{J}_{N-1}, \quad \text{(A30)}$$

where $\alpha = \omega_{\rm int}$ and $\beta = (\omega_t - \omega_{\rm int})/N$, and using the closed algebra,

$$\mathbb{J}_{N-1}\,\mathbb{J}_{N-1} = (N-1)\,\mathbb{J}_{N-1},$$

$$\mathbb{J}_{N-1}\,\mathbb{I}_{N-1} = \mathbb{I}_{N-1}\,\mathbb{J}_{N-1} = \mathbb{J}_{N-1},$$

$$\mathbb{I}_{N-1}\,\mathbb{I}_{N-1} = \mathbb{I}_{N-1}, \quad \text{(A31)}$$

we obtain

$$\boldsymbol{U}^{-1} = (\alpha \mathbb{I}_{N-1} + \beta \mathbb{J}_{N-1})^{-1} = \frac{1}{\alpha}\left(\mathbb{I}_{N-1} - \frac{\beta}{\alpha + (N-1)\beta}\mathbb{J}_{N-1}\right). \tag{A32}$$

So with $\boldsymbol{V}=\boldsymbol{I}_D$, one finds that

$$\boldsymbol{A}^{-1} = \frac{1}{\omega_{\text{int}}}\left(\mathbb{I}_{N-1} - \frac{(\omega_t - \omega_{\text{int}})}{(N-1)\omega_t + \omega_{\text{int}}}\mathbb{J}_{N-1}\right) \otimes \boldsymbol{I}_D. \tag{A33}$$

To evaluate $\det \boldsymbol{A}$ we note that

$$\det(\boldsymbol{U} \otimes \boldsymbol{V}) = (\det \boldsymbol{U})^{d_V}(\det \boldsymbol{V})^{d_U}, \tag{A34}$$

where d_U and d_V are the dimensionalities of matrices $\boldsymbol{U}$ and $\boldsymbol{V}$, respectively. The determinant of $\boldsymbol{I}_D$ is simple enough and equals unity. For $\det \boldsymbol{U}$ of Eq. (A30), we show that

$$\det \boldsymbol{U} = \det[\alpha \mathbb{I}_{N-1} + \beta \mathbb{J}_{N-1}] = \alpha^{(N-2)}[\alpha + (N-1)\beta]. \tag{A35}$$

Proof: We have

$$\det[\alpha \mathbb{I}_{N-1} + \beta \mathbb{J}_{N-1}] = \|\boldsymbol{E}\|, \tag{A36}$$

where $\boldsymbol{E}$ is the diagonal matrix of eigenvalues of $\boldsymbol{V}$ and $\|\boldsymbol{E}\|$ is the norm of $\boldsymbol{E}$, the product of its eigenvalues. Now since $\mathbb{J}_{N-1}=\mathbf{1}_c\mathbf{1}_c^T$, $\boldsymbol{x}_{N-1}=\frac{1}{\sqrt{N-1}}\mathbf{1}_c$ is seen to be a normalized eigenvector of $\boldsymbol{U}$ satisfying

$$\boldsymbol{U}\boldsymbol{x}_{N-1} = E_{N-1}\,\boldsymbol{x}_{N-1}, \tag{A37}$$

where

$$E_{N-1} = \alpha + (N-1)\beta. \tag{A38}$$

The remaining $N-2$ eigenvectors, $\boldsymbol{x}_j\ \forall\ \ 1 \le j \le N-2$, are orthogonal to $\boldsymbol{x}_{N-1}$ so $\mathbb{J}_{N-1}\boldsymbol{x}_j=0\ \forall\ \ 1 \le j \le N-2$, from which it follows that

$$\boldsymbol{U}\boldsymbol{x}_j = E_j\boldsymbol{x}_j, \tag{A39}$$

where

$$E_j = \alpha, \quad \forall \quad 1 \le j \le N-2. \tag{A40}$$

Putting it all together we arrive at Eq. (A35) (QED).

Using Eq. (A35) in Eq. (A34) we arrive at

$$\det \boldsymbol{A} = \alpha^{D(N-2)}\,[\alpha + (N-1)\beta]^D, \tag{A41}$$

$$= \frac{\omega_{\text{int}}^{D(N-2)}}{N^D}[(N-1)\omega_t + \omega_{\text{int}}]^D. \tag{A42}$$

As for $\exp(\boldsymbol{B}^T\boldsymbol{A}^{-1}\boldsymbol{B})$, Eqs. (A23) and (A33), along with

$$\mathbf{1}_c^T\,\mathbb{I}_{N-1}\,\mathbf{1}_c = (N-1), \tag{A43}$$

$$\mathbf{1}_c^T\,\mathbb{J}_{N-1}\,\mathbf{1}_c = (N-1)^2, \tag{A44}$$

give us

$$\exp(\boldsymbol{B}^T\boldsymbol{A}^{-1}\boldsymbol{B}) = \exp\left(\frac{(N-1)(\omega_t - \omega_{\text{int}})^2}{(N-1)\omega_t + \omega_{\text{int}}}\boldsymbol{r}^2\right). \tag{A45}$$

Thus from Eqs. (A29), (A41), and (A45) we obtain

$$M(r) = S(D)r^{D-1}\frac{\pi^{D(N-1)/2}\,N^{D/2}}{\sqrt{\omega_{\text{int}}^{D(N-2)}[(N-1)\omega_t + \omega_{\text{int}}]^D}}\exp(-\omega_{\text{eff}}\boldsymbol{r}^2), \tag{A46}$$

where

$$\omega_{\text{eff}} = \frac{N\omega_t\omega_{\text{int}}}{[\omega_{\text{int}} + (N-1)\omega_t]}. \tag{A47}$$

Finally using Eqs. (A20), (A46), and (A47) in Eq. (A12) we obtain

$$\mathcal{N}(r) = \frac{2N(\lambda_{\text{eff}}\omega_t)^{D/2}}{\Gamma\left(\frac{D}{2}\right)}\,r^{D-1}\exp(-\lambda_{\text{eff}}\,\omega_t\,r^2), \tag{A48}$$

where

$$\lambda_{\text{eff}} = \frac{N\omega_{\text{int}}}{\omega_{\text{int}} + (N-1)\omega_t} = \frac{1}{2\bar{r}_\infty^2}. \tag{A49}$$

Note that

$$\int_0^\infty \mathcal{N}(r)dr = N. \tag{A50}$$

3. Dimensional expansion of the number density

a. Dimensional scaling

To obtain the dimensional expansion of the density profile of Eq. (A48), we first need to regularize the large-dimension limit by dimensionally scaling the parameters and variables. As in Ref. [21], we define dimensionally scaled frequency $\bar{\omega}_t$ and the dimensionally scaled oscillator-scaled radial variable $\bar{r}$,

$$\bar{\omega}_t = D^3\omega_t, \tag{A51}$$

$$\bar{r} = \sqrt{\bar{\omega}_t}\frac{r}{D^2} = \sqrt{\frac{\omega_t}{D}}r, \tag{A52}$$

from which we derive

$$(\lambda_{\text{eff}}\,\omega_t)^{D/2}r^{D-1}dr = (\lambda_{\text{eff}}\,D)^{D/2}\bar{r}^{D-1}d\bar{r}. \tag{A53}$$

Thus the number density in dimensionally scaled coordinates is

$$\mathcal{N}(\bar{r}) = \frac{2N(\lambda_{\text{eff}}\,D)^{D/2}}{\Gamma\left(\frac{D}{2}\right)}\bar{r}^{D-1}\exp(-\lambda_{\text{eff}}\,D\bar{r}^2), \tag{A54}$$

where

$$\int_0^\infty \mathcal{N}(\bar{r})d\bar{r} = N. \tag{A55}$$

Equation (A54) implies [as does Eq. (A48)] that up to a scaling, the density profiles for harmonically interacting particles in a harmonic-confining potential follow a universal

curve for any N or interparticle interaction strength in oscillator units $\lambda_p \equiv \omega_p/\omega_t$, where

$$\lambda = \sqrt{1 + N\lambda_p^2} \quad \text{and} \quad \lambda_{\text{eff}} = \frac{N\lambda}{N + \lambda - 1}. \tag{A56}$$

This is simply seen by scaling the dimensionally scaled radius $\bar{r}$

$$\bar{r}_{\text{eff}} = \sqrt{\lambda_{\text{eff}}}\,\bar{r} \tag{A57}$$

and scaling the wave function by the multiplier $1/\sqrt{\lambda_{\text{eff}}}$ from the change of variables

$$d\bar{r} = \frac{1}{\sqrt{\lambda_{\text{eff}}}}\, d\bar{r}_{\text{eff}}, \tag{A58}$$

which gives the equation for the universal curve of the density profile as

$$\mathcal{N}(\bar{r}_{\text{eff}}) = \frac{2ND^{D/2}}{\Gamma\left(\frac{D}{2}\right)}\, \bar{r}_{\text{eff}}^{D-1}\, \exp(-D\bar{r}_{\text{eff}}^2), \tag{A59}$$

where

$$\int_0^\infty \mathcal{N}(\bar{r}_{\text{eff}})\, d\bar{r}_{\text{eff}} = N. \tag{A60}$$

As $D \to \infty$, the number density of Eq. (A54) becomes more and more strongly peaked at $(\bar{r}_{\text{eff}})_\infty$ determined from

$$\left.\frac{d\mathcal{N}(\bar{r}_{\text{eff}})}{d\bar{r}_{\text{eff}}}\right|_{D\to\infty} = 0, \tag{A61}$$

and thus the peak of the number density occurs precisely at the large-D radius parameter,

$$(\bar{r}_{\text{eff}})_\infty = \frac{1}{\sqrt{2}}. \tag{A62}$$

b. Series expansion

As in Ref. [21], we introduce the dimensionally scaled displacement coordinate

$$\bar{r}_{\text{eff}} = (\boldsymbol{r}_{\text{eff}})_\infty + \delta^{1/2}\, \bar{r}'_{\text{eff}} = \frac{1}{D^{1/2}}\, [\bar{r}'_{\text{eff}} + D^{1/2}\, (\bar{r}_{\text{eff}})_\infty] \tag{A63}$$

so that

$$d\bar{r}_{\text{eff}} = \frac{1}{D^{1/2}}\, d\bar{r}'_{\text{eff}}. \tag{A64}$$

Thus

$$\mathcal{N}(\bar{r}'_{\text{eff}}) = \frac{2N}{\Gamma\left(\frac{D}{2}\right)} [\bar{r}'_{\text{eff}} + D^{1/2}\, (\bar{r}_{\text{eff}})_\infty]^{D-1} \times \exp[-\,(\bar{r}'_{\text{eff}} + D^{1/2}\, (\bar{r}_{\text{eff}})_\infty)^2], \tag{A65}$$

where

$$\int_{-\sqrt{D}(\bar{r}_{\text{eff}})_\infty}^\infty \mathcal{N}(\bar{r}'_{\text{eff}})\, d\bar{r}'_{\text{eff}} = N. \tag{A66}$$

To derive the dimensional expansion of Eq. (A65), let us first consider expanding $[\bar{r}'_{\text{eff}} + D^{1/2}(\bar{r}_{\text{eff}})_\infty]^{D-1}$. We derive

$$[\bar{r}'_{\text{eff}} + D^{1/2}(\bar{r}_{\text{eff}})_\infty]^{D-1} = \left(\frac{D}{2}\right)^{(D-1)/2} \left[1 + \delta^{1/2}\left(\frac{\bar{r}'^3_{\text{eff}}}{3(\bar{r}_{\text{eff}})_\infty^3} - \frac{\bar{r}'_{\text{eff}}}{(\bar{r}_{\text{eff}})_\infty}\right) + O(\delta)\right] \times \exp\left(\frac{D^{1/2}\bar{r}'_{\text{eff}}}{(\bar{r}_{\text{eff}})_\infty}\right)\exp(-\bar{r}'^2_{\text{eff}}). \tag{A67}$$

Likewise we also have

$$\exp\{-[\bar{r}'_{\text{eff}} + D^{1/2}\,(\bar{r}_{\text{eff}})_\infty]^2\} = \exp\left(-\frac{D}{2}\right)\exp\left(-D^{1/2}\frac{\bar{r}'_{\text{eff}}}{(\bar{r}_{\text{eff}})_\infty}\right)\exp(-\bar{r}'^2_{\text{eff}}). \tag{A68}$$

Equations (A62), (A67), and (A68), along with

$$\sqrt{\frac{1}{\Gamma\left(\frac{D}{2}\right)}} = \frac{2^{(D-2)/4}\exp\left(\frac{D}{4}\right)}{\sqrt[4]{\pi}D^{(D-1)/4}} + O(\delta), \tag{A69}$$

give us the result we are after, namely,

$$\mathcal{N}(\bar{r}'_{\text{eff}}) = N\left[1 + \delta^{1/2}\sqrt{2}\left(\frac{2\bar{r}'^3_{\text{eff}}}{3} - \bar{r}'_{\text{eff}}\right) + O(\delta)\right]\left(\frac{2}{\pi}\right)^{1/2} \times \exp(-2\bar{r}'^2_{\text{eff}}), \tag{A70}$$

where through order $\delta^{1/2}$ the normalization condition

$$\int_{-\infty}^\infty \mathcal{N}(\bar{r}'_{\text{eff}}) d\bar{r}'_{\text{eff}} = N. \tag{A71}$$

is still satisfied.

As we noted after Eq. (A55), the density profile for harmonically interacting particles in a harmonic-confining potential follows a universal curve for any N or interparticle interaction strength $\lambda_p = \omega_p/\omega_t$. Although the density profile has this property, the same cannot be said for the wave function for N harmonically interacting particles in a harmonic-confining potential. For example, many terms in the wave function through first order in $\delta^{1/2}$ [see Eqs. (24)–(26) in Ref. [25]) are zero for the free trap ($\lambda_p = 0 \to \lambda = 1 \to \lambda_{\text{eff}} = 1$, $\bar{r}_\infty = 1/\sqrt{2}$, and $\gamma_\infty = 0$). Thus there is no simple scaling between the wave function for noninteracting particles in a harmonic-confining potential and the wave function for harmonically interacting particles in a harmonic-confining potential.

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