Analytic, Group-Theoretic Wave Functions for Confined $N$-Body Quantum Systems

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INTRODUCTION

During the last two decades, novel $N$-body quantum systems have been created using techniques to confine and manipulate atoms, ions, and electrons. These systems, of both fundamental and technological interest, include condensed atomic Bose gases, atoms confined in optical lattices, quantum dots, and ultracold fermion gases. Tuning the external fields of these environments provides unique opportunities to study many-body effects over a range of interaction strengths.

Mean-field treatments, such as the Hartree-Fock method in atomic physics and the Gross-Pitaevskii method in condensed matter, do not include correlation effects and fail to describe systems with tight confinement or strong interaction. These systems, which have hundreds to millions of particles, present serious challenges for existing $N$-body methods, many of which were developed with small systems in mind.

The methodology described below uses dimensional perturbation theory (DPT)\cite{1}, which has been previously applied to mostly small-$N$ systems in the form of high-order, largely numeric calculations. In this letter, we use group theoretic techniques to develop an analytic approach which fully exploits the symmetry of the zeroth-order problem. This method avoids heavy numerical computation, and $N$ enters into the theory as a parameter. This crucial simplification allows results for any $N$ to be obtained in a single calculation. This method also directly accounts for each two-body interaction, rather than using an average interaction. Even lowest-order results include beyond-mean-field effects. Thus, in contrast to the low-density expansion methods pioneered by Lee, Huang and Yang in the 1950s\cite{2}, this method is appropriate for the study of both weakly and strongly interacting systems and the transition between them. This general formalism offers a systematic approach to the study of correlation in atomic and molecular, condensed-matter, chemical, and nuclear systems.

Nearly all past work using DPT has focused on energies with little attention given to wave functions. In this paper we derive an analytic, correlated lowest-order $S$-wave wave function for $N$ identical particles in a spherical confining potential. The lowest-order wave function yields important information such as the nature of excitations and expectation values of physical observables. This result can be systematically improved by going to higher order.

TOOLBOX

The tools used to describe large-$N$ correlated wave functions are carefully chosen to maximize the use of symmetry and minimize the dependence on numerical computation. We handle the massive number of interactions for $N$ large ($\sim N^2/2$ two-body interactions) by bringing together three theoretical methods.

The first, DPT$^1$, is chosen because its zeroth-order equation, which is obtained for large $D$, yields a maximally-symmetric configuration for $N$ identical particles. Higher orders yield insight into fundamental motions as well as a framework for successive approximations. The second method is the FG method of Wilson, Decius, and Cross$^2$. This seminal method has long been used in quantum chemistry to study vibrations of polyatomic molecules. It directly relates the structure of the Schrödinger equation to the coordinate set which describes the normal modes of the system. The third method, the use of group theoretic techniques$^3$, takes full advantage of the symmetry at zeroth-order.

Dimensional Perturbation Theory

For $N$-body systems in large dimensions, the DPT wave function is localized about a symmetric structure in which each particle is equidistant and equiangular from every other particle. The Jacobian-weighted DPT wave function is harmonic and corresponds to oscillations about this structure. Notwithstanding its relatively simple form, the large-dimension, zeroth-order wave function

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\begin{align*}
\end{align*}
includes beyond-mean-field effects.

The Schrödinger equation for the zeroth-order Jacobian-weighted wave function has the form,

$$\left(-\frac{1}{2} \partial_{\bar{y}}^T G \partial_{\bar{y}} + \frac{1}{2} \bar{y}^T \mathbf{F} \bar{y} + v_0\right) \Phi_0(\bar{y}') = \Xi_0 \Phi_0(\bar{y}'),$$

(1)

where \(\bar{y}'\) is the displacement coordinate vector formed from dimensionally scaled internal displacement coordinates \(\bar{r}_i'\) (1 \(\leq i \leq N\)) and \(\bar{\gamma}_{ij}\) (1 \(\leq i < j \leq N\)). Coordinates \(\bar{r}_i'\) and \(\bar{\gamma}_{ij}\) are related to the \(D\)-dimensional scalar radii \(r_i\) of the \(N\) particles from the center of the confining potential and the cosines \(\gamma_{ij}\) of the \(N(N-1)/2\) angles between the radial vectors by

$$r_i = \kappa(D) \left(\bar{r}_\infty + \delta^{1/2} \bar{r}_i'\right), \quad \text{and} \quad \gamma_{ij} = \bar{\gamma}_\infty + \delta^{1/2} \bar{\gamma}_{ij}. $$

(2)

The expansion parameter is \(\delta = 1/D\), and \(\kappa(D)\) is quadratic in \(D\) with the particular form chosen to simplify the resulting equations. The quantities \(\bar{\gamma}_\infty\) and \(\bar{\gamma}_\infty\) define the symmetric large-dimension structure, which depends on the nature and strength of the interparticle interaction and confining potential. The matrices \(\mathbf{G}\) and \(\mathbf{F}\) are constants derived from the Hamiltonian.

The FG Method

The FG method is used to obtain normal-mode coordinates and frequencies from the eigenvalue problem in Eq. (1). The \(b\)th normal-mode coordinate \(q'_b\) may be written as

$$[q'_b] = b^T \bar{y}', \quad \text{where} \quad \mathbf{F} \mathbf{G} b = \lambda_b b, \quad \mathbf{b}^T \mathbf{G} b = 1, \quad \lambda_b = \tilde{\omega}_b^2, $$

(3)

and \(\tilde{\omega}_b\) is the normal-mode frequency. Equation (3) still represents a formidable eigenvalue problem unless \(N\) is quite small, since there are \(P = N(N+1)/2\) normal coordinates and up to \(P\) distinct frequencies.

Group Theory: the \(S_N\) Symmetry

The full \(S\)-wave Hamiltonian is invariant under particle interchange. This fact defines an \(S_N\) symmetry under which the system is invariant. As defined in Eq. (2), the large-dimension structure is a completely symmetric configuration so Eq. (1) is also invariant under the group \(S_N\). This \(S_N\) symmetry brings about a remarkable reduction from \(P\) possible distinct frequencies to five actual distinct frequencies and greatly simplifies the determination of the normal coordinates through the use of symmetry coordinates.

As a prelude to the above, we note that the \(S_N\) invariance of Eq. (1) means that the \(\mathbf{F}, \mathbf{G}\) and \(\mathbf{FG}\) matrices of Eq. (3) are invariant under \(S_N\), which implies that the eigenvectors \(b\) and normal modes transform under irreducible representations (irreps.) of \(S_N\). Using the theory of group characters, the coordinates \(\bar{r}_i'\) are reduced to one 1-dimensional and one \((N-1)\)-dimensional irrep., labelled \([N]\) and \([N-1, 1]\) respectively. The \(\bar{\gamma}_{ij}\) are reducible to one 1-dimensional, one \((N-1)\)-dimensional, and one \(N(N-3)/2\)-dimensional irrep., labelled \([N]\), \([N-1, 1]\), and \([N-2, 2]\) respectively. Since the normal modes transform under irreps. of \(S_N\) and are composed of linear combinations of elements of vectors \(\bar{r}'\) and \(\bar{\gamma}\), there will be two 1-dimensional, two \((N-1)\)-dimensional, and one entirely angular \(N(N-3)/2\)-dimensional irreps. labelled by the partitions \([N]\), \([N-1, 1]\) and \([N-2, 2]\) respectively. All normal modes that transform together under the same irrep. have the same frequency, so rather than \(P\) distinct frequencies there are only five!

NORMAL MODES – THE PROGRAM

We determine the normal coordinates and distinct frequencies in a three-step process:

First, we define sets of primitive irreducible coordinates that have the simplest possible functional form subject to the requirement that they transform under particular non-orthogonal irreps. of \(S_N\). We define two sets of linear combinations of elements of the \(\bar{r}'\) vector which transform under non-orthogonal \([N]\) and \([N-1, 1]\) irreps. of \(S_N\). We then derive two sets of linear combinations of elements of the \(\bar{\gamma}\) vector which transform under exactly these same two irreps. of \(S_N\). Finally we define a set of linear combinations of elements of \(\bar{\gamma}\) which transform under a particular non-orthogonal \([N-2, 2]\) irrep. of \(S_N\).

Second, we use linear combinations within each set of primitive irreducible coordinates to determine symmetry coordinates that are defined to transform under orthogonal irreps. of \(S_N\). Care is taken to ensure that this transformation to the symmetry coordinates preserves the identity of equivalent representations in the \(\bar{r}'\) and \(\bar{\gamma}\) sectors. We choose one of the symmetry coordinates to be a single primitive irreducible coordinate, the simplest functional form possible that transforms irreducibly under \(S_N\). The next symmetry coordinate is chosen to be composed of two primitive irreducible coordinates, and so on. Thus the complexity of the symmetry coordinates is minimized, building up slowly as symmetry coordinates are added.

Third, the \(\mathbf{FG}\) matrix, which was originally expressed in the \(\bar{r}'\) and \(\bar{\gamma}\) basis, is now expressed in symmetry coordinates. This results in a stunning simplification. The \(P \times P\) eigenvalue equation of Eq. (3) is reduced to one \(2 \times 2\) eigenvalue equation for the \([N]\) sector, \(N-1\) identical \(2 \times 2\) eigenvalue equations for the \([N-1, 1]\) sector,
and \(N(N-3)/2\) identical 1 \(\times\) 1 eigenvalue equations for the \([N-2,2]\) sector. For the \([N]\) and \([N-1,1]\) sectors, the 2 \(\times\) 2 structure allows for mixing of the \(\vec{r}'\) and \(\vec{r}\) symmetry coordinates in the normal coordinates (see Eq. (6) below). The 1 \(\times\) 1 structure of the equations in the \([N-2,2]\) sector reflects the absence of \(\vec{r}'\) symmetry coordinates in this sector, i.e. the \([N-2,2]\) normal modes are entirely angular.

The Symmetry Coordinates.

Using steps one and two, we derive the symmetry coordinates

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

where \(1 \leq i \leq N-1\), and

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

where \(1 \leq i \leq j-3\) and \(i+3 \leq j \leq N\).

The Normal Coordinates.

In the third step, Eq. (4) is expressed in the symmetry coordinate basis of Eq. (1) and reduces to three eigensystem equations (\(\alpha = [N], [N-1], [N-2,2]\)):

\[
\sigma^F G c^\alpha = \lambda^\alpha c^\alpha, \quad \text{and} \quad [c^\alpha]^T \sigma^G G c^\alpha = 1. \quad (5)
\]

The reduced \(G\) matrices \(\sigma^F G\) and \(\sigma^F G_{[N-1,1]}\) are 2 \(\times\) 2 matrices, while \(\sigma^F G_{[N-2,2]}\) is a 1 \(\times\) 1 matrix. The same is true for the diagonal reduced \(G\) matrices, \(\sigma^G G\). The elements of \(\sigma^F G\) and \(\sigma^G G\) are known analytic functions.\(^{[3]}\)

There are five solutions to Eq. (4) denoted \(0^\pm = \{\lambda^{[N]}_\pm, c^{[N]}_\pm\}, \quad 1^\pm = \{\lambda^{[N-1,1]}_\pm, c^{[N-1,1]}_\pm\}\) and \(2^\pm = \{\lambda^{[N-2,2]}_\pm, c^{[N-2,2]}_\pm\}\). The two-element \(c^\alpha\) vectors for the \(\alpha = [N]\) and \([N-1,1]\) sectors determine the angular-radial mixing of the symmetry coordinates in a normal coordinate of a particular \(\alpha\). Hence

\[
[q']_b = [c^N_\alpha]_\Gamma [S^{[N]}_{\gamma'}]_\xi + [c^{[N-1,1]}_\alpha]_\Gamma [S^{[N-1,1]}_{\gamma'}]_\xi + [c^{[N-2,2]}_\alpha]_\Gamma [S^{[N-2,2]}_{\gamma'}]_\xi. \quad (6)
\]

The normal coordinate label \(b\) is replaced by the labels \(\alpha\), \(\xi\) and \(\pm\) on the rhs of Eq. (6). For the \([N-2,2]\) sector, the symmetry coordinates are also the normal coordinates up to a normalization constant, \([c^{[N-2,2]}]=[S^{[N-2,2]}_\gamma]\).

The Wave Function.

The wave function in Eq. (1) is the product of \(P\) harmonic-oscillator wave functions:

\[
\Phi_0(\vec{r}') = \prod_{\mu=0^\pm, 1^\pm} \prod_{\xi=1}^{d_\mu} \phi_n^{(\mu)}(\sqrt{\omega_\mu} [q'^\mu]_\xi), \quad (7)
\]

where \(\phi_n^{(\mu)}(\sqrt{\omega_\mu} [q'^\mu]_\xi)\) is a one-dimensional harmonic-oscillator wave function of frequency \(\omega_\mu\), and \(n_\mu\) is the oscillator quantum number, \(0 \leq n_\mu < \infty\), which counts the number of quanta in each normal mode. The quantity \(\mu\) labels the manifold of normal modes with the same frequency \(\omega_\mu\) while \(d_\mu = 1\), \(N - 1\) or \(N(N-3)/2\) for \(\mu = 0^\pm\), \(1^\pm\) or \(2\) respectively.

UNMASKING THE WAVE FUNCTION: THE DENSITY PROFILE

In the case of macroscopic quantum-confined systems, such as a BEC, the wave function is made manifest in the experimentally accessible density profile.

The large-dimension Jacobian-weighted ground-state density profile, \(N_0(r)\), is an analytic function:
The analytic DPT density profile of Eq. (9) is a Gaussian, symmetric about $\kappa(D)\bar{r}_\infty$. For $a$ or $N$ sufficiently large, the physical density profile develops an asymmetry which motivates future work on the next-order DPT wavefunction.

**SUMMARY AND CONCLUSIONS**

This letter discusses an analytic approach to the study of quantum-confined $N$-body systems. Unlike mean-field methods, this approach directly accounts for each interparticle interaction, even at lowest-order, and so is applicable to high-density, strongly-interacting systems. By taking advantage of three powerful methods, DPT, the FG method and the group theory of the $SN$ group, we avoid heavy numerical computation and offer a systematic approach to correlation that is not limited to small-$N$ systems. While most prior work with DPT has focused on energies, this letter derives the lowest-order, analytic, correlated wave function for a spherically-confined, $N$-particle system and the corresponding analytic density profile.

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