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Nightingale Replies:

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Nightingale Replies: The focus of Ref. [1] was the computation of excited states of identical symmetry. The wave functions were explicitly designed for the symmetry of the ground state of identical spinless bosons, a state invariant under translation and both proper and improper rotations. Indeed, the fact that the wave functions are functions only of interparticle distances makes this obvious as far as the spatial symmetries are concerned. For details pertaining to particle exchange see Ref. [2].

Although one cannot compute pseudoscalar states with the trial functions of Ref. [1], this is not a fundamental limitation; suitable trial functions can be found. I appreciate the opportunity to clarify matters presented in the preceding Comment [3], and shall devote the rest of this Reply to how pseudoscalar states can be constructed. Without actual computation it is impossible to know the accuracy of the results of the suggested generalization. The general rule seems to be that as states develop more structure, the accuracy that can be obtained decreases rapidly, but we do not expect that low-lying pseudoscalar states will pose a serious problem.

Consider a system of n particles in d dimensions. We use the position representation with particles at positions $\mathbf{r}_1, \ldots, \mathbf{r}_n$. For states of vanishing total momentum one can, without loss of generality, choose trial functions that are linear combinations of *elementary basis* functions of the form $\psi = \zeta\{\mathbf{r}_{1j}\}\eta\{r_{ij}\}$, where $\{\mathbf{r}_{1j}\}$ denotes dependence on all interparticle *vectors* $\mathbf{r}_{ij} = \mathbf{r}_j - \mathbf{r}_i$ with $i = 1 < j$; $\{r_{ij}\}$ is the same for the interparticle *distances* with $i < j$.

A straightforward generalization of the approach used in Ref. [1], the function ζ is assumed to be a homogeneous, pseudoscalar multinomial in the $\mathbf{r}_{1j}$, minimal in the sense that it is constructed by symmetrization of a monomial in these variables. Consequently, it has no variable coefficients, other than a single overall factor fixed by convention.

For the sake of argument, assume that the factor $\eta\{r_{ij}\}$ is some simple function that imposes short- and long-range boundary conditions on the wave function. In practice, η contains nonlinear parameters that can be adjusted to obtain better trial functions.

Any scalar ζ that is a multinomial in the Cartesian coordinates of n vectors can be written a multinomial in $\mathbf{r}_{1i} \cdot \mathbf{r}_{1j}$ [4]. Any such pseudoscalar ζ can be obtained as a sum of determinants of the matrices column k of which is $\mathbf{r}_{1i_k}$. Denote these determinants by D_α, where α runs through all possible choices of $2 \le i_k \le n$, $k = 1, \ldots, n$ with $i_1 < i_2 < \cdots < i_d$. Then $\zeta = \sum_\alpha p_\alpha D_\alpha$ with scalar multinomials p_α. No powers of the D_α appear because the product of two determinants D_α and D_β is a scalar, the determinant of a matrix of inner products $\mathbf{r}_{1i} \cdot \mathbf{r}_{1j}$. It immediately follows that in d dimensions there are no translationally invariant pseudoscalar wave functions for fewer then $d + 1$ particles.

D_α is antisymmetric in d coordinate indices and symmetric in the rest. If each p_α behaves the same way as D_α, the resulting ζ will be bosonic. To write ζ as a multinomial of fundamental invariants we construct a set of such invariants, algebraically complete to the highest degree desired in the computation. For the scalar case we used the following algorithm. Generate a list of all possible homogeneous multinomials of increasing degree up to some order. Symmetrize each monomial and remove duplicates; order the list with increasing degree and increasing complexity for each degree. To generate a basis of fundamental invariants iteratively, go through this list and check if a given invariant can be written as a sum of powers of previously found fundamental invariants; if not, add this invariant to the basis. This calculation only has to be done once and in the cases we have dealt with can be done to higher order than is needed for the computations. Whether the basis is complete or not, although perhaps interesting from a mathematical point of view, is not of practical interest. It should, however, be noted, as mentioned in Ref. [2], that syzygies may exist that render the optimization parameters linearly dependent. To generalize this algorithm to pseudoscalars, one has to take into account that there will be pseudoscalar fundamental invariants and that each term in the multinomial will contain precisely one such quantity multiplied by a multinomial of scalar fundamental invariants.

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