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Permutation Symmetry in Spin Adapted Many-Body Wave Functions

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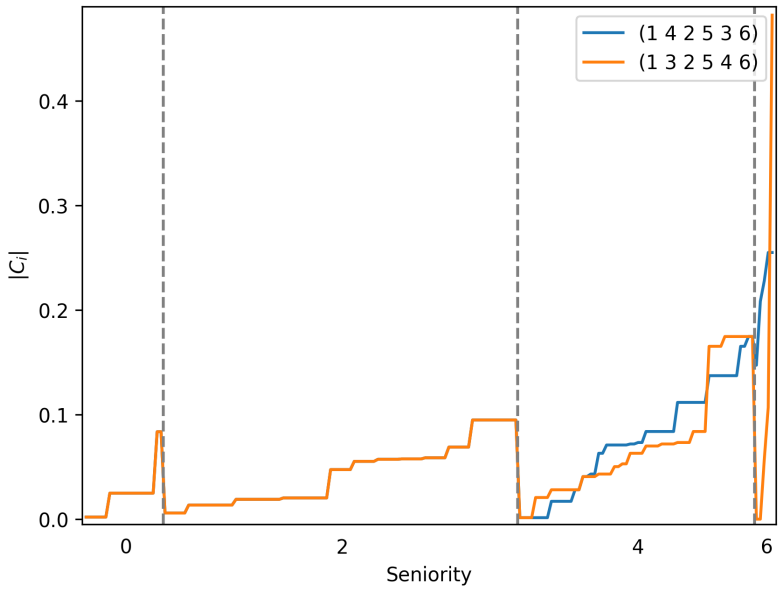

Fig. 1 Absolute values of the GUGA CI vectors of a (6e, 6o) benzene cluster using (142536) and (132546) orderings. The cluster consists of localized $2p_z$ orbitals. CSFs are classified by their seniority and different seniority blocks are distinguished by vertical dashed lines. Within the seniority-4 block, the L_4 norms of (142536) and (132546) orderings are 0.3003 and 0.3243, respectively. The L_4 norms of (142536) and (132546) within the seniority-6 block are 0.3408 and 0.4823, respectively.

Table 1 Symmetry Non-Equivalent Site Orderings and Corresponding L_4-Norms[a] for two 4-Site Rhombus Clusters with $S_{\text{loc}} = 1/2$

Sym. Elem.	Symmetry Non-Equivalent Site Orderings					
E	1234	2314	2341	1243	1324	2413
$C_2(z)$	3412	4132	4123	3421	3142	4231
$C_2(y)$	1432	4312	4321	1423	1342	4213
$C_2(x)$	3214	2134	2143	3241	3124	2431
$L_4(S_{\text{tot}} = 0)$	0.889	0.889	0.889	0.889	**1.000**	**1.000**
$L_4(S_{\text{tot}} = 1)$	0.847	0.847	0.889	0.889	0.863	**1.000**

[a] *L_4-norm calculated from the CI eigenvectors for each site ordering.*
[b] We use $J_{12} = J_{23} = J_{34} = J_{14} = -1.789$, $J_{13} = -1.000$, and $J_{24} = -2.000$.

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Table 2 Symmetry Non-Equivalent Site Orderings and Corresponding L_4-Norms[a] for a 4-Site Kite Cluster with $S_{\mathsf{loc}} = 1/2$

Sym. Elem.	Symmetry Non-Equivalent Site Orderings											
E	2314	3412	4132	1234	4123	1243	2341	3421	1324	3142	4231	2413
$C_2(z)$	4312	3214	2134	1432	2143	1423	4321	3241	1342	3124	2431	4213
$L_4(S_{\mathrm{tot}} = 0)$	0.889	0.889	0.889	0.889	0.889	0.889	0.889	0.889	**1.000**	**1.000**	**1.000**	**1.000**
$L_4(S_{\mathrm{tot}} = 1)$	0.835	0.835	0.886	0.886	0.888	0.888	0.925	0.925	0.779	0.779	0.928	**0.998**

[a] *L_4-norm calculated from the CI eigenvectors for each site ordering.*
[b] We use $J_{12} = J_{14} = -1.638$, $J_{23} = J_{34} = -0.894$, $J_{13} = -0.741$, and $J_{24} = -1.000$.

Table 3 Symmetry Non-Equivalent Site Orderings and Corresponding L_4-Norms[a] for a 4-Site Irregular Tetrahedron Cluster with $S_{\mathsf{loc}} = 1/2$

Sym. Elem.	Symmetry Non-Equivalent Site Orderings											
E	1342	1432	3142	4132	1324	1423	3124	4123	3412	4312	1234	1243
σ	2341	2431	3241	4231	2314	2413	3214	4213	3421	4321	2134	2143
$L_4(S_{\mathrm{tot}} = 0)$	0.889	0.889	0.889	0.889	0.889	0.889	0.889	0.889	**1.000**	**1.000**	**1.000**	**1.000**
$L_4(S_{\mathrm{tot}} = 1)$	0.847	0.847	0.847	0.847	0.889	0.889	0.889	0.889	0.863	0.863	**1.000**	**1.000**

[a] *L_4-norm calculated from the CI eigenvectors for each site ordering.*
[b] *We use $J_{12} = -6.770$, $J_{13} = J23 = -4.320$, and $J_{14} = J_{24} = J_{34} = -3.140$.*

Table 4 Symmetry Non-Equivalent Site Orderings and Corresponding L_4-Norms[a] for a 4-Site Irregular Tetrahedron Cluster with $S_{\mathsf{loc}} = 3/2$

Sym. Elem.	Symmetry Non-Equivalent Site Orderings											
E	1342	1432	3142	4132	1324	1423	3124	4123	3412	4312	1234	1243
σ	2341	2431	3241	4231	2314	2413	3214	4213	3421	4321	2134	2143
$L_4(S_{\mathrm{tot}} = 0)$	0.681	0.681	0.681	0.681	0.681	0.681	0.681	0.681	**1.00**	**1.000**	**1.000**	**1.000**
$L_4(S_{\mathrm{tot}} = 1)$	0.470	0.470	0.470	0.470	0.546	0.546	0.546	0.546	0.581	0.581	**0.802**	**0.802**
$L_4(S_{\mathrm{tot}} = 3)$	0.613	0.613	0.613	0.613	0.681	0.681	0.681	0.681	0.636	0.636	**1.000**	**1.000**

[a] *L_4-norm calculated from the CI eigenvectors for each site ordering.*
[b] *We use $J_{12} = -6.770$, $J_{13} = J23 = -4.320$, and $J_{14} = J_{24} = J_{34} = -3.140$.*

Table 5 Symmetry Non-Equivalent Site Orderings and Corresponding L_4-Norms[a] for a 6-Site Hexagon Cluster with $S_{\mathsf{loc}} = 3/2$

Sym. Elem.	Symmetry Non-Equivalent Site Orderings									
E	142536	143625	142563	143652	142365	143256	142356	143265	124536	125463
$L_4(S_{\mathrm{tot}} = 0)$	0.291605	0.291605	0.291605	0.291605	0.416236	0.416236	0.416236	0.416236	0.416236	0.416236
$L_4(S_{\mathrm{tot}} = 1)$	0.219767	0.219767	0.219773	0.219773	0.276694	0.276694	0.278434	0.278434	0.318175	0.318175
$L_4(S_{\mathrm{tot}} = 2)$	0.192944	0.192944	0.192956	0.192956	0.208708	0.208708	0.213273	0.213273	0.280617	0.280617
$L_4(S_{\mathrm{tot}} = 3)$	0.189795	0.189795	0.189813	0.189813	0.187739	0.187739	0.194028	0.194028	0.272746	0.272746
$L_4(S_{\mathrm{tot}} = 4)$	0.191527	0.191527	0.191607	0.191607	0.190432	0.190432	0.195471	0.195471	0.236338	0.236338
E	124563	125436	123645	126354	123654	126345	123465	126534	123456	126543
$L_4(S_{\mathrm{tot}} = 0)$	0.416236	0.416236	0.431538	0.431538	0.431538	0.431538	0.468135	0.468135	0.468135	0.468135
$L_4(S_{\mathrm{tot}} = 1)$	0.318179	0.318179	0.292137	0.292137	0.293135	0.293135	0.331733	0.331733	0.324428	0.324428
$L_4(S_{\mathrm{tot}} = 2)$	0.280635	0.280635	0.224665	0.224665	0.227524	0.227524	0.265640	0.265640	0.245845	0.245845
$L_4(S_{\mathrm{tot}} = 3)$	0.272756	0.272756	0.201068	0.201068	0.205700	0.205700	0.232805	0.232805	0.213734	0.213734
$L_4(S_{\mathrm{tot}} = 4)$	0.236554	0.236554	0.197559	0.197559	0.202504	0.202504	0.217486	0.217486	0.207280	0.207280
E	142635	143526	134652	136452	134625	136425	142653	143562	124356	125643
$L_4(S_{\mathrm{tot}} = 0)$	0.471383	0.471383	0.471383	0.471383	0.471383	0.471383	0.471383	0.471383	0.480340	0.480340
$L_4(S_{\mathrm{tot}} = 1)$	0.332913	0.332913	0.355124	0.355124	0.355128	0.355128	0.337523	0.337523	0.331241	0.331241
$L_4(S_{\mathrm{tot}} = 2)$	0.257797	0.257797	0.307266	0.307266	0.307280	0.307280	0.264773	0.264773	0.251096	0.251096
$L_4(S_{\mathrm{tot}} = 3)$	0.224646	0.224646	0.293867	0.293867	0.293879	0.293879	0.231316	0.231316	0.216035	0.216035
$L_4(S_{\mathrm{tot}} = 4)$	0.219303	0.219303	0.278047	0.278047	0.278153	0.278153	0.224180	0.224180	0.206298	0.206298
E	124365	125634	134265	136245	124635	125364	124653	125346	134256	136254
$L_4(S_{\mathrm{tot}} = 0)$	0.480340	0.480340	0.632198	0.632198	0.632198	0.632198	0.632198	0.632198	0.632198	0.632198
$L_4(S_{\mathrm{tot}} = 1)$	0.339496	0.339496	0.423450	0.423450	0.427328	0.427328	0.459971	0.459971	0.430079	0.430079
$L_4(S_{\mathrm{tot}} = 2)$	0.270617	0.270617	0.311060	0.311060	0.312347	0.312347	0.365193	0.365193	0.325974	0.325974
$L_4(S_{\mathrm{tot}} = 3)$	0.235881	0.235881	0.268057	0.268057	0.257556	0.257556	0.309530	0.309530	0.281832	0.281832
$L_4(S_{\mathrm{tot}} = 4)$	0.217332	0.217332	0.258340	0.258340	0.238293	0.238293	0.269477	0.269477	0.267279	0.267279
E	132456	132654	123564	126435	132465	132645	123546	126453	134526	136524
$L_4(S_{\mathrm{tot}} = 0)$	0.648718	0.648718	0.648718	0.648718	0.648718	0.648718	0.648718	0.648718	0.762381	0.762381
$L_4(S_{\mathrm{tot}} = 1)$	0.437035	0.437035	0.439802	0.439802	0.443763	0.443763	0.468612	0.468612	0.527784	0.527784
$L_4(S_{\mathrm{tot}} = 2)$	0.319355	0.319355	0.321913	0.321913	0.338498	0.338498	0.369095	0.369095	0.392766	0.392766
$L_4(S_{\mathrm{tot}} = 3)$	0.268387	0.268387	0.264519	0.264519	0.291311	0.291311	0.311348	0.311348	0.324011	0.324011
$L_4(S_{\mathrm{tot}} = 4)$	0.253824	0.253824	0.242747	0.242747	0.269766	0.269766	0.270352	0.270352	0.296710	0.296710
E	134562	136542	135426	135624	135462	135642	135246	135264	132546	132564
$L_4(S_{\mathrm{tot}} = 0)$	0.762381	0.762381	0.903035	0.903035	0.903035	0.903035	0.903265	0.903265	**0.942394**	**0.942394**
$L_4(S_{\mathrm{tot}} = 1)$	0.547272	0.547272	0.631282	0.631282	0.631344	0.631344	0.631353	0.631353	**0.650726**	**0.650726**
$L_4(S_{\mathrm{tot}} = 2)$	0.424058	0.424058	0.470572	0.470572	0.470672	0.470672	0.470556	0.470556	**0.473444**	**0.473444**
$L_4(S_{\mathrm{tot}} = 3)$	0.354116	0.354116	**0.381139**	**0.381139**	0.381073	0.381073	0.381019	0.381019	0.370511	0.370511
$L_4(S_{\mathrm{tot}} = 4)$	0.319076	0.319076	**0.338540**	**0.338540**	0.338478	0.338478	0.338517	0.338517	0.318171	0.318171

[a] *L_4-norm calculated from the CI eigenvectors for each site ordering.*
[b] *We use $J_{12} = J_{23} = J_{34} = J_{45} = J_{56} = J_{16} = -6.700$, $J_{13} = J_{24} = J_{35} = J_{46} = J_{15} = J_{26} = -3.500$, and $J_{14} = J_{25} = J_{36} = -3.100$.*