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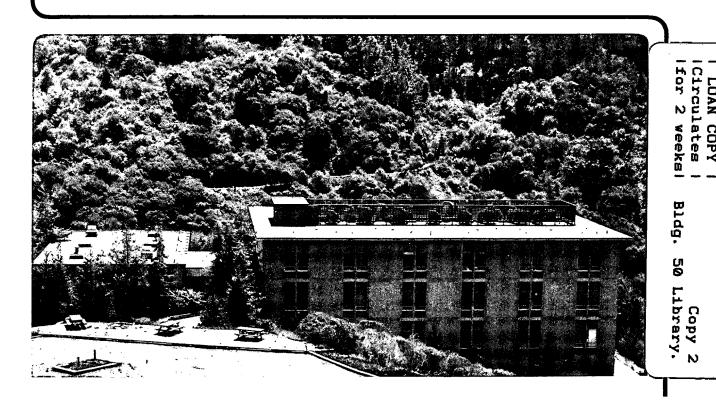## UNIVERSITY OF CALIFORNIA

Materials & Chemical Sciences Division

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HIDDEN SYMMETRIES OF FINITE-SIZE CLUSTERS
WITH PERIODIC BOUNDARY CONDITIONS*

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ABSTRACT

Finite-size clusters with periodic boundary conditions resemble isolated clusters for a small number of sites and infinite lattices for a large number of sites. The transition from the small, self-contained system (point-group regime) to an infinite lattice (space-group regime) passes through an intermediate region with increased (hidden) symmetry. In this high-symmetry regime the translation subgroup is not an invariant subgroup of the whole group, and irreducible representations of the space group may stick together to form higher-dimensional representations of the complete symmetry group. In addition to explaining some puzzling accidental degeneracies, the enlarged symmetry group has important implications in small-cluster studies and in numerical simulations.

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The periodic crystal approximation[1] is the fundamental approximation for study-
ing bulk properties of solid-state systems. It has been used quite successfully in
band-structure calculations,[2] Monte-Carlo simulations,[3] and the small-cluster approach
to the many-body problem.[4] In the periodic crystal approximation a crystal of M sites
is modeled by a lattice of M sites with periodic boundary conditions (PBC). Bloch's
theorem[5] then labels the quantum-mechanical wavefunctions by one of M wavevectors
in the Brillouin zone. In principle, the thermodynamic limit ($M \rightarrow \infty$) is then taken,
which replaces the finite grid in reciprocal space by a continuum that spans the Bril-
louin zone. In practice, the number of lattice sites is chosen to be as large as possible
(M = finite), and the solution of the quantum-mechanical problem corresponds to a
finite sampling in reciprocal space.

In the thermodynamic limit the complete symmetry group of the lattice is the
space group, which is composed of all translations, rotations, and reflections that
(rigidly) map the lattice onto itself and preserve its neighbor structure. In the case of a
finite cluster, the complete symmetry group is a subgroup of S_M, the permutation
group of M elements, and is called the cluster-permutation group. The cluster-
permutation group may (A) be a proper subgroup of the space group (*i.e.* it has fewer
elements than the space group), (B) contain operations that are not elements of the

space group, or (C) be identical to the space group. These three regimes are called, respectively, (A) the self-contained-cluster regime, (B) the high-symmetry regime, and (C) the lattice regime. Note that the space group need not be a subgroup of the cluster-permutation group in the high-symmetry regime (although it usually is).

The lattice-regime clusters appear for large enough M, assuming that the unit cell is chosen with enough symmetry. In this regime (C) the group properties are completely determined by the space group, and the irreducible representations are labeled by a k-vector in the Brillouin zone and (at symmetry planes, lines and points) by a subindex that determines the relevant irreducible representation[6] of the small group of k.

A self-contained cluster (A) is a cluster essentially identical to an isolated, box-boundary-conditions cluster. The addition of PBC adds no new connections between lattice sites, but merely renormalizes parameters in the Hamiltonian. In this case, the cluster-permutation group is *identical* to the symmetry group of the same isolated cluster. This symmetry group is a point group, not necessarily the full point group of the lattice. It has its origin at a particular point (generally *not* a lattice point) called the center of the cluster; it is a proper subgroup of the space group. This isomorphism was first observed in the four-site square (sq) and tetrahedral (face-centered cubic, fcc) clusters[7] and in the eight-site simple-cubic (sc) cluster.[8] The regime where the cluster-permutation group is a subgroup of the space group is called the self-contained-cluster regime since every known example occurs in self-contained clusters.

The four-site sq-lattice cluster is an example of a self-contained cluster. The lattice sites lie on the corners of an elemental square and are numbered from one to four in a clockwise direction. The neighbor structure, with PBC, is such that the four first-nearest-neighbors (1NN) of an odd-numbered (even-numbered) site are *two* each of the even-numbered (odd-numbered) sites, and the four second-nearest neighbors (2NN) are *four* each of remaining odd-numbered (even-numbered) site. Therefore, the isolated

four-atom square and the PBC four-site square lattice are identical if the 1NN interactions are renormalized by a factor of two and 2NN interactions by a factor of four. Note that the imposition of PBC does not add any new connections to the lattice. The cluster-permutation group is the point group C_{4v} with an origin at the center of the square; it is a proper subgroup (order 8) of the space group (order 32). It should be noted in passing that the complete neighbor structure for the four-site PBC sq-lattice cluster is fully determined by labeling only the 1NNs. Lattices that can be defined by the 1NN structure alone are called 1NN-determined lattices; all known examples of self-contained clusters are 1NN-determined lattices.

For intermediate-size clusters there are additional permutation operations that leave the Hamiltonian invariant. They either (non-rigidly) map the lattice onto itself and preserve the entire neighbor structure of the lattice,[9] or (for short-range-interaction Hamiltonians) they preserve *only* the 1NN structure of the lattice. The size of the cluster-permutation group may be much larger than the space group in this case (B).

The transition from (A) self-contained cluster to (B) high-symmetry cluster, to (C) lattice is illustrated in Tables I and II for the simplest set of sc, bcc, fcc, and sq lattice clusters: the set whose number of sites is a power of two ($M = 2^j$). These sets can all be constructed with maximum cubic or square symmetry, with the exception of the $M = 2$ cluster for the fcc lattice. Table I corresponds to arbitrary Hamiltonians; Table II, to 1NN-interaction only. The self-contained-cluster regime (A) corresponds to $M \leq 8$ ($M \leq 4$) for the sc lattice (otherwise). The high-symmetry regime (B) is present at intermediate values of M: for example, $16 \leq M \leq 64$ for the sc lattice; $8 \leq M \leq 32$ for the bcc lattice; and $8 \leq M \leq 16$ for the fcc and sq lattices when the Hamiltonian contains only 1NN interactions (see Table II). The lattice regime (C) is entered for larger cluster sizes. The cluster-permutation group (in the high-symmetry regime) has been studied for some specific clusters.[10-12]

It is interesting to note that the fcc lattice is the only lattice that has the same symmetry for general Hamiltonians and 1NN-only interactions. This fact probably arises because the fcc lattice is not bipartite.[13]

In the self-contained-cluster regime, the cluster-permutation group is a proper subgroup of the space group, because some space-group operations are redundant (*i.e.*, identical to the identity operation). The redundancy implies that only a *subset* of the irreducible representations of the space group (those that represent the redundant operations by the unit matrix) are accessible to the solutions of the Hamiltonian. This process of rigorously eliminating irreducible representations as acceptable representations is well known. It occurs, for example, in systems that possess inversion symmetry: if the basis functions are inversion symmetric, then the system sustains only representations that are even under inversion. A typical example of this property[7] is the four-site tetrahedral fcc cluster. The space group is of order 192 and has 20 irreducible representations: 10 with k-vector at the center of the Brillouin zone Γ, and 10 with k vector at the center X of the square faces. The redundant operations are the three twofold rotations about the x-, y-, and z-axes and the inversion, all centered at lattice points. The cluster-permutation group is isomorphic to the tetrahedral point group T_d, with 24 elements and 5 irreducible representations. Of the 20 representations of the space group, only Γ_1, Γ_2, Γ_{12}, X_1, and X_2 survive.

In the high-symmetry regime (B), the cluster-permutation group contains operations that are not elements of the space group. The set H of elements of the cluster-permutation group G that are elements of the space group forms a subgroup of the cluster-permutation group that, usually, is equal to the space group. The group of translations T forms an abelian invariant subgroup of H so that Bloch's theorem holds. The irreducible representations of H are all irreducible representations of the space group. When the full cluster-permutation group G is considered, the class structure of H is expanded and modified, in general, with classes of H combining together,

and/or elements of G outside H uniting with elements in a class of H, to form the new class structure of the cluster-permutation group G. The classes that contain the set of translations typically contain elements that are not translations, so that the translation subgroup is no longer an invariant subgroup and representations of the cluster-permutation group cannot be constructed in the standard way.[14] Furthermore, every irreducible representation of H that has nonuniform characters for the set of classes of H that have combined to form one class of G must combine with other irreducible representations to form a higher-dimensional irreducible representation of the cluster-permutation group. This phenomenon can be interpreted as a *sticking together* of irreducible representations of the space group arising from the extra (hidden) symmetry of the cluster.

One example of the high-symmetry regime is the eight-site cluster in the fcc-lattice. The space group contains 384 elements, divided into 26 classes. The points in the fcc Brillouin zone sampled[6] here are Γ, X, and L. The full cluster-permutation group G contains also 384 elements. The inversion, however, is a redundant operation; there are therefore only 192 elements of G which are ordinary space-group operations: the subgroup H of translations and proper rotations. This subgroup contains the following 13 irreducible representations (with their corresponding dimensions in parentheses): Γ_1 (1), Γ_2 (1), Γ_{12} (2), Γ_{15}' (3), Γ_{25}' (3), X_1 (3), X_2 (3), X_3 (3), X_4 (3), X_5 (6), L_1 (4), L_2 (4), and L_3 (8). The full character table is well known.[8] There is in addition one permutation (and the corresponding operations required by closure), which involves the interchange of *one single pair* of 2NNs, that leaves the Hamiltonian invariant. This extra permutation completely modifies the class structure: there are now only 20 classes in G. Of the corresponding 20 irreducible representations 18 reduce, in the absence of the new permutation, to single, well defined representations of H, two to each of the following: Γ_1, Γ_2, Γ_{12}, X_1, X_2, X_5, L_1, L_2, and L_3. There are, in addition, two six-dimensional representations that "violate" Bloch's theorem:

one that reduces to $\Gamma_{15}' \oplus X_4$, the other to $\Gamma_{25}' \oplus X_3$. Put in different terms, the "hidden" extra symmetry has two major effects: (1) it separates the Hamiltonian matrix blocks of nine representations of the space group into two irreducible blocks each; and (2) four the other four it causes two pairs of irreducible representations at two different points in the Brillouin zone to "stick together".

The additional symmetry here is the explanation for several "mysterious" degeneracies found, either numerically or analytically, in many cluster calculations. This "sticking together" of the states was even more puzzling because it involved states with different translational symmetry. Even though the wavefunction can still be written as Bloch states, the irreducible representation of the full group requires, in some cases, Bloch states of different k-vector. Moreover, the extra symmetry may result in great simplifications of the numerical problems when diagonalizing matrices and, as has been the case in the past,[15] result in problems with completely analytical solutions.

From the practical point of view three effects may make this extra symmetry particularly useful: The groups may be extremely large (see for example the group of order 7,962,624 for the 16-site cluster in the fcc-lattice); the size of the cluster may be fairly large before this extra symmetry is lost (it survives up to the 64-site cluster in the sc-lattice with 1NN-only interactions); and it is even more pronounced in systems with short-range-only interactions (compare Tables I and II; the 16-site bcc-lattice cluster with 1NN-only interactions has a cluster-permutation group of order 3,251,404,800), making the property more useful for some of the systems of great current interest.[16]

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Table I. Order of the space and the cluster-permutation groups for arbitrary interactions on finite-size clusters with periodic boundary conditions of the simple, body-centered, and face-centered cubic lattices and of the two-dimensional square lattice. The symbols A, B, and C denote the self-contained, high-symmetry, and lattice regimes, respectively. The cases with cluster sizes larger than 32 are in the lattice regime (C).

cluster size	cubic space group	sc		bcc		fcc		square space group	sq	
1	48	A	1	A	1	A	1	8	A	1
2	96	A	2	A	2	–	–	16	A	2
4	192	A	24	A	8	A	24	32	A	8
8	384	A	48	B	1,152	B	384	64	B	128
16	768	B	12,288	B	4,608	B	7,962,624	128	C	128
32	1,536	C	1,536	C	1,536	C	1,536	256	C	256

Table II. Order of the space and the cluster-permutation groups for 1NN-only interactions on finite-size clusters with periodic boundary conditions of the simple, body-centered, and face-centered cubic lattices and of the two-dimensional square lattice. The symbols A, B, and C denote the self-contained, high-symmetry, and lattice regimes, respectively. The cases with cluster sizes larger than 128 are in the lattice regime (C).

cluster size	cubic space group	*sc*		*bcc*		*fcc*		square space group	*sq*	
1	48	A	1	A	1	A	1	8	A	1
2	96	A	2	A	2	–	–	16	A	2
4	192	A	24	A	8	A	24	32	A	8
8	384	A	48	B	1,152	B	384	64	B	1,152
16	768	B	12,288	B	3,251,404,800	B	7,962,624	128	B	384
32	1,536	B	13,824	B	6,144	C	1,536	256	C	256
64	3,072	B	27,648	C	3,072	C	3,072	512	C	512
128	6,144	C	6,144	C	6,144	C	6,144	1,024	C	1,024

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