

## Enlarged Symmetry Groups of Finite-Size Clusters with Periodic Boundary Conditions

J. K. FREERICKS and L. M. FALICOV

*Department of Physics, University of California, Berkeley, CA 94720, U.S.A. and  
Materials Sciences Division, Lawrence Berkeley Laboratory, Berkeley,  
CA 94720, U.S.A.*

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**Abstract.** Any system that approximates an infinite lattice by a family of finite clusters (with periodic boundary conditions) passes through an intermediate region with enlarged (hidden) symmetry as the system size is increased. The hidden symmetry allows for extra degeneracies and level crossings and has application to exact-diagonalization studies, Monte Carlo simulations, lattice gauge theories, and renormalization group calculations.

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The periodic crystal approximation [1] is the fundamental approximation for studying 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 [6]. 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 Brillouin zone (or equivalently replaces the finite cluster by an infinite lattice in real space). In practice, the number of lattice sites is chosen to be as large as possible ( $M = \text{finite}$ ), and the solution of the quantum-mechanical problem corresponds to a finite sampling in reciprocal space. It should be emphasized that *every* calculation that samples at only a finite number of points in reciprocal space corresponds to a finite-cluster with periodic boundary conditions in real space.

Realistic models of physical systems (that incorporate many-body interactions on the same footing as single-particle interactions) can be analyzed for only the smallest systems. Recent examples include calculations of the photoemission spectra [7] of nickel ( $M = 4$ ), structural properties [8] of diamond and silicon ( $M = 8$ ), and x-ray absorption spectra [9] in high-temperature superconducting oxides ( $M = 10$ ). It is not known, in general, how large a finite system must be to capture the relevant physics of a real system (in the thermodynamic limit). Group theory can be used to address this question by identifying when extra symmetries of finite clusters (with

periodic boundary conditions) exist and by analyzing the representation theory of these enlarged groups. Group theory is a rigorous and model-independent tool that determines when particular matrix elements are required to be, e.g., identical or zero. Such analysis leads to two possible finite-size effects of the hidden symmetry when compared to the standard analysis based upon the space group: energy levels can 'stick together' and/or 'violate' the no-crossing rule.

A finite cluster with PBCs can be viewed as a mapping of an infinite lattice onto  $M$  equivalence classes – each class corresponding to a different site of the cluster [10] (for example, any bipartite [11] lattice of translationally equivalent sublattices can be represented by a two-site cluster with the  $\alpha$  sublattice corresponding to equivalence class one and the  $\beta$  sublattice corresponding to equivalence class two). The lattice contains only  $M$  inequivalent translations since any translation that does not change the equivalence classes of the sites is made identical to the null translation (for example, the two-site cluster has two translations; the first corresponds to the null translation and carries sublattice  $\alpha \rightarrow \alpha$  and sublattice  $\beta \rightarrow \beta$ ; while the second corresponds to the translation from one site to the other and carries sublattice  $\alpha \leftarrow \rightarrow \beta$ ). The neighbor structure of the lattice is determined by the successive nearest-neighbor shell (on-site, first-nearest-neighbor, second-nearest-neighbor, *etc.*) that exhaust all  $M$  equivalence classes (the two-site cluster contains only on-site and, normally, first-nearest-neighbor shells). Note that each neighbor shell may contain members of an equivalence class *more than once* (if the bipartite lattice has  $Z$  nearest neighbors then the nearest neighbors on site one are  $Z$  atoms of equivalence class two). The space group is finite and consists of  $Mh$  elements, where  $h$  is the number of elements in the point group (the largest value for  $h$  is 48 for cubic lattices; it is 8 for square lattices).

In the thermodynamic limit ( $M \rightarrow \infty$ ) the complete symmetry group of the lattice is the (infinite) space group (with  $Mh$  elements), which is composed of all translations, rotations, and reflections that (rigidly) map the infinite 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 the  $M$  cluster sites, and is called the cluster-permutation group. The cluster-permutation group, which contains *all* operations that leave the Hamiltonian invariant, may (A) be a proper subgroup of the (finite) space group (i.e. it has fewer elements than the space group), (B) contain operations that are not elements of the (finite) space group, or (C) be identical to the (finite) 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 whole (finite) space group need not be a subgroup of the cluster-permutation group in the high-symmetry regime (although it usually is).

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 the neighbor structure of the cluster with PBCs may contain multiples of the neighbor structure of the isolated cluster (thereby renor-

malizing parameters in the Hamiltonian in going from one to the other). 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 is a proper subgroup of the space group. This isomorphism was first observed [10, 12] in the  $2 \times 2$  square (*sq*) and the four-site tetrahedral (face-centered cubic, *fcc*) clusters ( $M = 4$ ) and in the  $2 \times 2 \times 2$  simple-cubic (*sc*) cluster ( $M = 8$ ).

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., there is a group homomorphism between the space group and the cluster permutation group with a nontrivial kernel). The redundancy implies that only a *sub-set* of the irreducible representations of the space group (those that represent the elements of the kernel 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 those representations that are even under inversion.

For intermediate-size clusters there are additional permutation operations that leave the Hamiltonian invariant. They either (nonrigidly) map the lattice onto itself and preserve the entire neighbor structure of the lattice, or (for short-range-interaction Hamiltonians) they preserve *only* the first-nearest neighbor (1NN) structure of the lattice [13]. These hidden symmetry operations may expand the cluster-permutation group to a group that is (much) larger than the (finite) space group.

The group theory for the cluster-permutation group in the high-symmetry regime (B) may be analyzed as follows. 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 [14]. The group of translations  $T$  forms an Abelian invariant subgroup of  $H$ ; 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 [15]. 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 (i.e., the subgroup  $H$ ) arising from the extra (hidden) symmetry of the cluster.

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

Table I. Number of symmetry elements in the space and the cluster-permutation groups (CPG) 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 all in the lattice regime (C).

Cluster size	Space group cubic	CPG						Space group square	CPG	
		<i>sc</i>		<i>bcc</i>		<i>fcc</i>			<i>sq</i>	
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	1152	B	384	64	B	128
16	768	B	12 288	B	4608	B	7 962 624	128	C	128
32	1536	C	1536	C	1536	C	1536	256	C	256

completely determined by the space group, and the irreducible representations are labeled by a wavevector in the Brillouin zone and (at symmetry planes, lines and points) by a subindex that determines the relevant irreducible representation [16] under rotations and reflections. The wavevector  $\mathbf{k}$  labels the characters of the Abelian invariant subgroup of translations by determining the phase change  $\exp(i\mathbf{k} \cdot \boldsymbol{\tau})$  for a translation  $\boldsymbol{\tau}$  (Bloch's theorem).

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 cubic (*sc*, *bcc*, and *fcc*) and square (*sq*) lattice clusters: the set whose number of sites is a power of two ( $M = 2^l$ ). These sets can all be constructed with maximum cubic or square symmetry, with the exception of the  $M = 2$  cluster for the *fcc* lattice. The tables record the sizes of the space group and the cluster-permutation group for the chosen set of clusters. Table I corresponds to arbitrary Hamiltonians; Table II, to

Table II. Number of symmetry elements in the space and the cluster-permutation groups (CPG) for INN-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 all in the lattice regime (C).

Cluster size	Space group cubic	CPG						Space group square	CPG	
		<i>sc</i>		<i>bcc</i>		<i>fcc</i>			<i>sq</i>	
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	1152	B	384	64	B	1152
16	768	B	12 288	B	3 251 404 800	B	7 962 624	128	B	384
32	1536	B	13 824	B	6144	C	1536	256	C	256
64	3072	B	27 648	C	3072	C	3072	512	C	512
128	6144	C	6144	C	6144	C	6144	1024	C	1024

Hamiltonians with only 1NN-interactions. Notice that for (A) the number of elements in the cluster-permutation group  $n_{\text{CPG}}$  is *always* smaller than in the space group  $n_s$ ; for (B) usually  $n_{\text{CPG}} > n_s$ , although it is possible to have  $n_{\text{CPG}} = n_s$  (see Table I, *fcc* cluster of 8 sites); for (C) *always*  $n_{\text{CPG}} = n_s$ . 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, when the Hamiltonian contains only 1NN interactions the high-symmetry regime appears for  $16 \leq M \leq 64$  in the *sc* lattice;  $8 \leq M \leq 32$  in the *bcc* lattice; and  $8 \leq M \leq 16$  in the *fcc* and *sq* lattices (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 [17–19].

As an example, the transition from a self-contained cluster to the lattice regime can be examined in more detail for the *fcc* lattice. The four-site tetrahedral *fcc* cluster is a self-contained cluster (see Figure 1). The nearest neighbors of each site of the tetrahedron are the other three sites. The imposition of PBCs produces an *fcc* lattice (see Figure 1a) in which each of the four interpenetrating *sc* sublattices of the *fcc* lattice is assigned to a different equivalence class. The twelve nearest neighbors of each site are now *four* atoms of each of the other three equivalence classes (see Figure 1b). The only difference between the tetrahedral cluster with box boundary conditions (representing an isolated tetrahedron) and the tetrahedral cluster with periodic boundary conditions (representing an *fcc* lattice) is the 1NN interactions in the Hamiltonian are renormalized by a factor of four in the latter case. The space group is of order 192 ( $4 \times 48$ ) and has 20 irreducible representations: 10 with wavevector at the center of the Brillouin zone  $\Gamma$   $\{\mathbf{k} = [0, 0, 0]\}$ , and 10 with wavevector at the center  $X$   $\{\mathbf{k} = [\pi, 0, 0], \mathbf{k} = [0, \pi, 0], \mathbf{k} = [0, 0, \pi]\}$  of the square

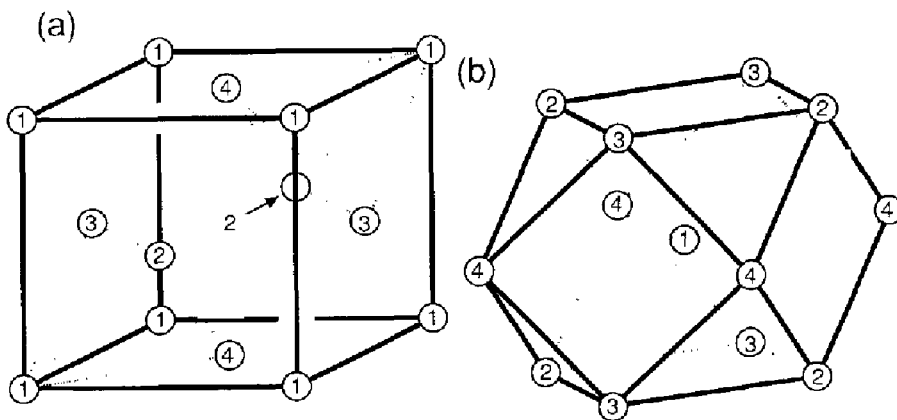


Fig. 1. Four site *fcc* cluster. (a) The distribution of sites in cubic unit cell in real space. (b) The labeling (equivalence class) of the twelve nearest neighbors of a site of class 1; they are four sites of class 2, four of class 3, and four of class 4. It can be seen that (i) inversion leaves the cluster invariant (identity operation) and (ii) so does a two-fold rotation about axes which pass through site 1 and join two opposite centers of the square faces of the polyhedron.

faces (representations at  $\Gamma$  are unchanged by any translation, at  $X$  they change sign for two of the three nonzero translations). The kernel of the group homomorphism (that maps the space group onto the cluster-permutation group) consists of the three twofold rotations about the  $x$ -,  $y$ -, and  $z$ -axes and the inversion with all operations centered at lattice points (see Figure 1b). 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 groups, only  $\Gamma_1\langle A_1 \rangle$ ,  $\Gamma_2\langle A_2 \rangle$ ,  $\Gamma_{12}\langle E \rangle$ ,  $X_1\langle T_1 \rangle$ , and  $X_2\langle T_2 \rangle$  survive, where the space-group notation is that of reference 16, and the angular brackets indicate the standard [1] labeling of the representations of  $T_d$ .

The eight-site cluster in the *fcc*-lattice is constructed by doubling the primitive unit cell of the *fcc* lattice and is in the high-symmetry regime (see Figure 2). The space group contains 384 ( $8 \times 48$ ) elements divided into 26 classes. The wavevectors in the *fcc* Brillouin zone sampled [16] here are

$$\Gamma \quad \{\mathbf{k} = [0, 0, 0]\}, \quad X \quad \{\mathbf{k} = [\pi, 0, 0], \mathbf{k} = [0, \pi, 0], \mathbf{k} = [0, 0, \pi]\}$$

and

$$L \quad \{\mathbf{k} = [\pi/2, \pi/2, \pi/2], \mathbf{k} = [\pi/2, -\pi/2, -\pi/2], \mathbf{k} = [-\pi/2, \pi/2, -\pi/2], \\ \mathbf{k} = [-\pi/2, -\pi/2, \pi/2]\}.$$

The full cluster-permutation group  $G$  contains also 384 elements. The inversion, however, is an operation that is identical to the identity (see Figure 2b); 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 [16] (with their corresponding dimensions in parentheses):  $\Gamma_1(1)$ ,  $\Gamma_2(1)$ ,  $\Gamma_{12}(2)$ ,  $\Gamma'_{15}(3)$ ,  $\Gamma'_{25}(3)$ ,  $X_1(3)$ ,  $X_2(3)$ ,  $X_3(3)$ ,  $X_4(3)$ ,

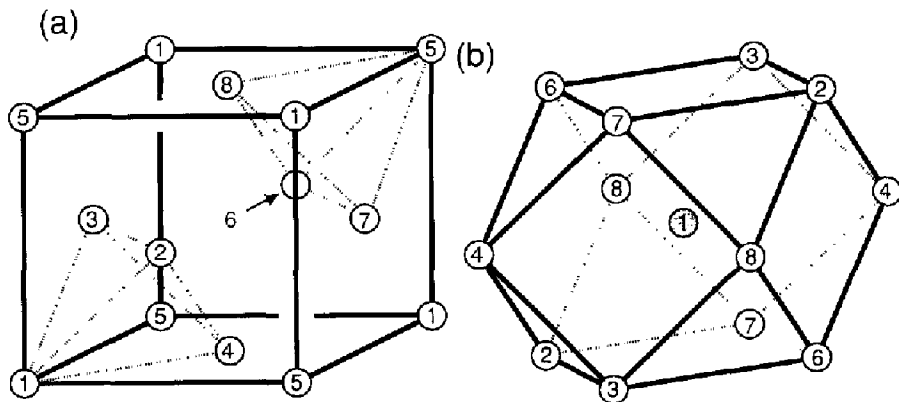


Fig. 2. Eight-site *fcc* cluster. (a) The distribution of sites in a cubic unit cell in real space. (b) The labeling (equivalence class) of the twelve nearest neighbors of a site of class 1; they are two sites each of classes 2, 3, 4, 6, 7, and 8. Six sites in class 5 constitute the second-nearest neighbors. It can be seen that inversion leaves the numbering unchanged, i.e. is homomorphic to the identity operation.

$X_5(6)$ ,  $L_1(4)$ ,  $L_2(4)$ , and  $L_3(8)$ . The full character table of the subgroup  $H$  is well known [10] and will not be repeated here. There is in addition one permutation  $P$  (and the corresponding operations required by closure), which involves the interchange of *one single pair* of 2NNs (for example, the interchange of sites 1 and 5 in Figure 2a), that leaves the Hamiltonian invariant. This permutation is a nonrigid operation that, although it maps the lattice onto itself, *cannot be constructed out of any rotation followed by a translation*. The cluster-permutation group contains 20 classes. 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 nine:  $\Gamma_1$ ,  $\Gamma_2$ ,  $\Gamma_{12}$ ,  $X_1$ ,  $X_2$ ,  $X_5$ ,  $L_1$ ,  $L_2$ , and  $L_3$ . There are, in addition, two six-dimensional representations that 'go beyond' (seem to 'violate') Bloch's theorem [20]: 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 subgroup  $H$  of the space group into two irreducible blocks each (corresponding to the irreducible representations of the cluster-permutation group  $G$ ); and (2) for the other four (representations of  $H$ ) it causes two pairs of representations at two different wavevectors in the Brillouin zone to 'stick together'.

The 16-site *fcc* cluster is also in the high-symmetry regime (B). It is constructed out of four interpenetrating *sc* sublattices with each *sc* sublattice composed of four inequivalent classes. The 1NNs of any site are one atom each of the twelve inequivalent classes that comprise the other three *sc* sublattices. The six 2NNs are two atoms each of the remaining three inequivalent classes of the original *sc* sublattice. Therefore, any permutation of the four elements within a *sc* sublattice or any permutation of the four *sc* sublattices will map the lattice onto itself and thereby commute with the Hamiltonian. The cluster-permutation group contains  $(4!)^4 = 7\,962\,624$  elements, and has a similar structure to the eight-site cluster-permutation group: it is a very large group and will not be analyzed in detail here. All larger clusters lie in the lattice regime (C) and analysis proceeds as usual.

The additional symmetry discussed here is the explanation for several 'mysterious' degeneracies found, either numerically or analytically, in cluster calculations [10, 12]. 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 a Bloch state, the irreducible representation of the full group requires, in some cases, Bloch states of different wavevectors. 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 [21], result in problems with completely analytical solutions. The additional symmetry may also explain why Monte Carlo simulations on  $4 \times 4$ ,  $6 \times 6$ , and  $8 \times 8$  square lattice clusters [22] show that the  $6 \times 6$  and  $8 \times 8$  clusters (which do not have any additional symmetry) approximate the thermodynamic limit much better than the  $4 \times 4$  (which is in the B regime).

From the practical point of view three effects make this extra symmetry particularly useful: The subgroups 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  $[4 \times 4 \times 4]$  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 3 241 404 800), making the property more useful for some of the systems of great current interest [23]. There may be a tradeoff in actual calculations between utilizing the full symmetry of the cluster-permutation group or just the symmetry of a convenient subgroup, however the solutions will reflect the effects of the *full* cluster-permutation group whether it is actually employed to reduce the Hamiltonian blocks or not.

In conclusion, it should be stressed that the presence of an enlarged symmetry group for moderately sized clusters is a finite-size effect that can be *rigorously* analyzed by the techniques of group theory. Furthermore, any attempt to extrapolate the results of a finite-cluster calculation to the thermodynamic limit must not possess the properties of the eigenstates that are required by the presence of these 'hidden' symmetry operations. Finally, note that although the phenomenon examined here is discussed in the context of exact-diagonalization studies of solid state systems, it will occur in any system that approximates an infinite lattice by a family of finite clusters and may have useful applications to Monte Carlo simulations [3], lattice-gauge theories [24], or real-space decimation calculations [25].

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