Hidden symmetries of finite-size clusters with periodic boundary conditions

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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 a self-contained system to an infinite lattice passes through an intermediate region with increased (hidden) symmetry. In this high-symmetry region irreducible representations of the space group may stick together to form higher-dimensional representations of the complete symmetry group. This transition is examined for a class of simple-, body-centered-, and face-centered-cubic lattice clusters and the two-dimensional square lattice cluster. The implications of an enlarged symmetry group are also studied for a model of strongly correlated electrons interacting on eight-site clusters.

I. INTRODUCTION

The fundamental approximation for studying bulk properties of solid-state systems is the periodic crystal approximation.[1] 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, an M-site crystal is modeled by a lattice of M sites[5] with periodic boundary conditions (PBC). Bloch's theorem[6] then labels the quantum-mechanical wave functions by one of M wave vectors in the Brillouin zone. In principle, a macroscopic crystal is studied by taking the thermodynamic limit ($M \rightarrow \infty$), which replaces the finite grid in reciprocal space by a continuum within the Brillouin 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 can be a proper subgroup of the space group (i.e., it has fewer elements than the space group), contain operations that are not elements of the space group, or be identical to the space group. These three regimes are called, respectively, the self-contained-cluster regime, the high-symmetry regime, and 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).

A self-contained cluster is a cluster that does not add any new connections between lattice sites when PBC are imposed, but merely renormalizes parameters in the Hamiltonian. In this case, the cluster-permutation group is *identical* to the symmetry group of the same cluster with box boundary conditions. This symmetry group is, in turn, a point group (not necessarily the full point group of the lattice) with its origin at some point which can be called the center of the cluster; it is a proper subgroup of the space group. This phenomenon was first observed in the four-site square and tetrahedral clusters[7] and in the eight-site simple-cubic 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 square-lattice cluster is an example of a self-contained cluster. The lattice sites of the isolated cluster lie on the corners of a square and are numbered 1–4 in a clockwise direction [see Fig. 1(a)]. When PBC are imposed (see Table I), the four first-nearest neighbors (1NN) of site 1 are *two* each of the sites 2 and 4 and the four second-nearest neighbors (2NN) are *four* each of site 3. Therefore, 1NN interactions must be renormalized by a factor of 2 and 2NN interactions by a factor of 4. Note that the imposition of PBC does not add any new connections to the lattice. The cluster-permutation group is isomorphic to the point group C_{4v} with an origin at the center of the square; the latter is a proper subgroup (order 8) of the space group (order 32).

The neighbor structure of a finite cluster is only defined to the full extent of the cluster; i.e., the neighbor structure includes the minimal set of neighbor shells that exhaust all of the sites of the cluster. The neighbor structure for the four-site square-lattice cluster is recorded in Table I. This information is, in fact, overcomplete since the entire lattice can be defined by the 1NN structure alone. Such a lattice is called a 1NN-determined lattice and all known examples of self-contained clusters are 1NN-determined lattices.

There are two ways to generate symmetry operations that are not elements of the space group yielding the high-symmetry regime. The first possibility is that the lattice is *not* a 1NN-determined lattice. In this case, there are always additional permutation operations that

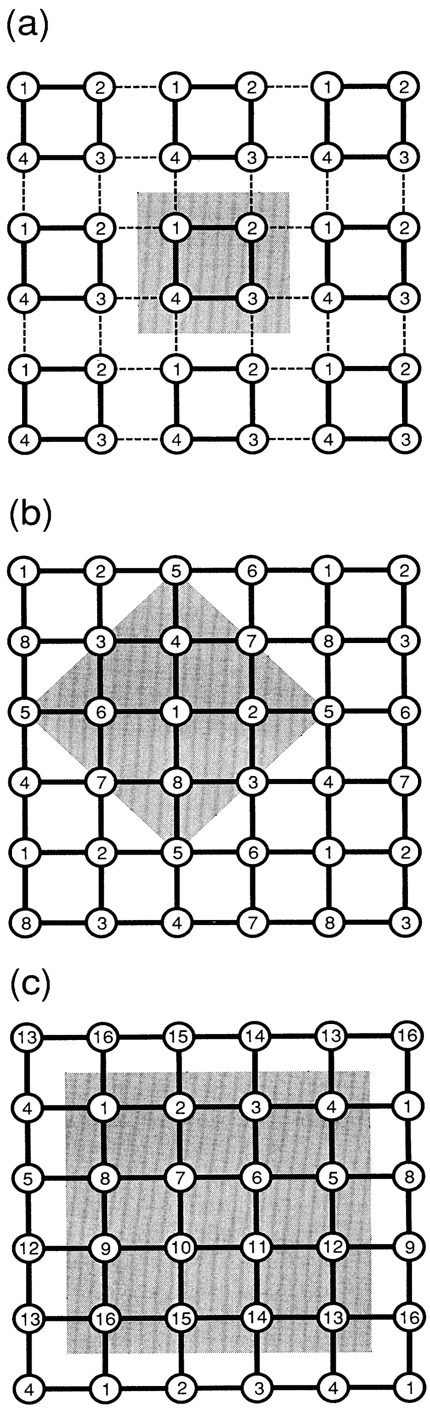

FIG. 1. Four-, eight-, and sixteen-site clusters with periodic boundary conditions in the square lattice. The $\sqrt{M}\times\sqrt{M}$ tilings of the square lattice are shaded. The four-site cluster [panel (a)] is a self-contained cluster since the periodic boundary conditions do not add any new lattice connections. This fact is highlighted by the dashed lines in (a). The eight-site cluster [panel (b)] is not a 1NN-determined lattice, as discussed in the text, and lies in the high-symmetry regime. The 16-site cluster [panel (c)] has no additional symmetry for arbitrary interactions, but does possess hidden symmetry for Hamiltonians that contain only 1NN interactions.

TABLE I. Neighbor structure for the four-site square lattice cluster.

Site	1NN				2NN			
1	2	2	4	4	3	3	3	3
2	1	1	3	3	4	4	4	4
3	2	2	4	4	1	1	1	1
4	1	1	3	3	2	2	2	2

(nonrigidly) map the lattice onto itself and preserve the entire neighbor structure of the lattice.[9] The size of the cluster-permutation group can be very large in this case. The second possibility occurs in a 1NN-determined lattice, but the extra symmetry operations preserve *only* the 1NN structure of the lattice.[10] A necessary (but not sufficient) condition for this phenomenon is given in the Appendix.

When the size of the cluster is large enough, the system enters the lattice regime with the cluster-permutation group identical to the space group. This always occurs because a large enough cluster is 1NN determined and does not satisfy the necessary condition for extra symmetry operations given in the Appendix.

This contribution examines the implications of these extra symmetry operations to the quantum-mechanical solutions of Hamiltonians defined on small clusters. In Sec. II, the transition from a self-contained system to an infinite lattice is studied for a class of cubic (and square) clusters and the consequences of the enlarged symmetry groups are outlined. Section III follows this transition in detail for a square-lattice system. Section IV studies the eight-site clusters for the simple-, body-centered-, and face-centered-cubic lattices and the square lattice. The group theory is applied to the many-body solutions of a model of strongly correlated electrons (the $t-t'-J$ model). Section V contains a summary of the results and a conclusion.

II. GROUP THEORY FOR CUBIC CLUSTERS

The transition from a self-contained cluster to a lattice is illustrated for the simplest set of simple- (sc), body-centered- (bcc), and face-centered- (fcc) cubic lattice clusters and the square (sq) lattice cluster: the set whose number of sites is a power of two ($M=2^j$). Note that a subset of clusters (those with sizes that correspond to j being a multiple of the spatial dimension of the lattice) are easily formed by repeatedly doubling the unit cell. For example, doubling the unit cell increases the cluster size by a factor of eight (four) for the cubic (square) systems.

The clusters for general j are constructed as follows. A sc lattice is composed of two interpenetrating fcc sublattices or four interpenetrating bcc sublattices. Similarly, a bcc (fcc) lattice is composed of two (four) interpenetrating sc sublattices. A small cluster with PBC is constructed by decomposing an infinite lattice into M interpenetrating sublattices (using the above decompositions) and assigning a different equivalence class (site number) to each of the M sublattices. For example, an eight-site fcc lattice cluster is constructed from four sc sublattices with each sc sublattice represented by two fcc sublattices (see Fig. 3 of Ref. 8). If each sc sublattice is represented by four bcc sublattices, a 16-site fcc lattice cluster is formed, and so on. The sq lattice clusters (see Fig. 1) are constructed from $\sqrt{M}\times\sqrt{M}$ tilings of the plane that are aligned with (rotated by 45° with respect to) the underlying square lattice for even (odd) j. In this fashion, every cluster whose number of sites is a power of 2 can be constructed except for the two-site fcc lattice cluster.

Tables II and III summarize the results for the order of the cluster-permutation groups of the sc, bcc, fcc, and sq lattice clusters as a function of cluster size. Table II corresponds to arbitrary Hamiltonians, and Table III to Hamiltonians with 1NN interactions only. The self-contained-cluster regime corresponds to $M\leq 8$ ($M\leq 4$) for the sc lattice (otherwise). The high-symmetry regime is present at intermediate values of M: For example, when the Hamiltonian contains only 1NN interactions, the high-symmetry regime appears at $16\leq M\leq 64$ 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 (see Table III). The lattice regime is entered for larger cluster sizes. The cluster-permutation group (in the high-symmetry regime) has been studied previously for sq lattice clusters.[11–13]

A size range always exists where the lattice is not a 1NN-determined lattice. In this case the order of the cluster-permutation group can be huge. For example, the 16-site fcc lattice is composed of four interpenetrating sc sublattices with each sc sublattice composed of four sites (four interpenetrating bcc sublattices). The 1NN of any site are the 12 sites that comprise the other three sc sublattices. The second-nearest neighbors (2NN) are the three remaining sites of the original sc sublattice (each counted twice). Therefore, any permutation of the four elements within a sc sublattice or any permutation of the four sc sublattices will commute with the Hamiltonian. The order of the cluster-permutation group is then $(4!)^5=7\,962\,624$.

There are many implications that result from a cluster-permutation group that is *not* identical to the space group. In the self-contained-cluster regime, the cluster-permutation group is a subgroup of the space group, because some space-group operations are redundant (identical to the identity operation). In other words, a homomorphism exists between the space group and the cluster-permutation group with a nontrivial kernel composed of the redundant operations. This 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.

In the high-symmetry regime, the cluster-permutation group G 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 is usually equal to the space group. The group of translations forms an Abelian invariant subgroup of H so that Bloch's theorem[6] 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 of 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 *sticking together* of irreducible representations of the space group arising from the extra (hidden) symmetry of the cluster.

There are further implications for short-ranged interactions. In the cases when the Hamiltonian has extra symmetry for 1NN-only interactions, the energy spectrum has levels that stick together in the absence of longer-ranged interactions and split as these interactions

TABLE II. Order of the cluster-permutation group 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 S, H, and L denote the self-contained, high-symmetry, and lattice regimes, respectively. The cases with cluster sizes larger than 32 are in the lattice regime.

Cluster size	Cubic space group		sc		bcc		fcc	Square space group		sq
1	48	S	1	S	1	S	1	8	S	1
2	96	S	2	S	2			16	S	2
4	192	S	24	S	8	S	24	32	S	8
8	384	S	48	H	1 152	H	384	64	H	128
16	768	H	12 288	H	4 608	H	7 962 624	128	L	128
32	1536	L	1 536	L	1 536	L	1 536	256	L	256

TABLE III. Order of the cluster-permutation group 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 S, H, and L denote the self-contained, high-symmetry, and lattice regimes, respectively. The cases with cluster sizes larger than 128 are in the lattice regime.

Cluster size	Cubic space group		sc		bcc		fcc	Square space group		sq
1	48	S	1	S	1	S	1	8	S	1
2	96	S	2	S	2			16	S	2
4	192	S	24	S	8	S	24	32	S	8
8	384	S	48	H	1 152	H	384	64	H	1152
16	768	H	12 288	H	3 251 404 800	H	7 962 624	128	H	384
32	1536	H	13 824	H	6 144	L	1 536	256	L	256
64	3 072	H	27 648	L	3 072	L	3 072	512	L	512
128	6144	L	6 144	L	6 144	L	6 144	1024	L	1024

are turned on. However, the solutions will be *nearly* degenerate if the longer-ranged interactions are "weak" in relation to the 1NN interactions.

III. EXAMPLE: THE SQUARE LATTICE

The transition from the self-contained-cluster regime, through the high-symmetry regime, to the lattice regime is illustrated for the sq lattice. The four-site sq lattice cluster [Fig. 1(a)] is a self-contained cluster. The space group is of order 32 and is composed of 14 classes. The Brillouin zone[15] is sampled at three symmetry stars: Γ $(d=1)$, M $(d=1)$, and X $(d=2)$. The origin of the space group is chosen to be site 1. One finds that the twofold rotation $\{C_4^2|0\}$, and the reflections about the x and y axes $\{\sigma_x|0\}$ and $\{\sigma_y|0\}$, are all redundant operations;

TABLE IV. Character table for the space group of the four-site cluster on the square lattice. The symbol σ denotes the mirror planes perpendicular to the x and y axes and σ' denotes the mirror planes perpendicular to the diagonals $x\pm y$. The translations are denoted by 0 (no translation), τ (first-nearest neighbor translation), and θ (second-nearest neighbor). The subscripts $\parallel$ and $\perp$ refer to translations parallel to or perpendicular to the normals of the mirror planes, respectively. The acceptable representations of the space group, which form the representations of the cluster-permutation group, are emboldened.

	1	1	2	1	1	2	4	4	2	2	2	2	4	4
	E	C_4^2	σ	E	C_4^2	σ	C_4	σ'	E	C_4^2	σ	σ	C_4	σ'
	0	0	0	θ	θ	θ	τ	τ	τ	τ	$\tau_\parallel$	$\tau_\perp$	0θ	0θ
$\mathbf{\Gamma_1}$	**1**	**1**	**1**	**1**	**1**	**1**	**1**	**1**	**1**	**1**	**1**	**1**	**1**	**1**
Γ_2	1	1	−1	1	1	−1	1	−1	1	1	−1	−1	1	−1
$\mathbf{\Gamma_3}$	**1**	**1**	**1**	**1**	**1**	**1**	**−1**	**−1**	**1**	**1**	**1**	**1**	**−1**	**−1**
Γ_4	1	1	−1	1	1	−1	−1	1	1	1	−1	−1	−1	1
Γ_5	2	−2	0	2	−2	0	0	0	2	−2	0	0	0	0
$\mathbf{M_1}$	**1**	**1**	**1**	**1**	**1**	**1**	**−1**	**−1**	**−1**	**−1**	**−1**	**−1**	**1**	**1**
M_2	1	1	−1	1	1	−1	−1	1	−1	−1	1	1	1	−1
$\mathbf{M_3}$	**1**	**1**	**1**	**1**	**1**	**1**	**1**	**1**	**−1**	**−1**	**−1**	**−1**	**−1**	**−1**
M_4	1	1	−1	1	1	−1	1	−1	−1	−1	1	1	−1	1
M_5	2	−2	0	2	−2	0	0	0	−2	2	0	0	0	0
$\mathbf{X_1}$	**2**	**2**	**2**	**−2**	**−2**	**−2**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
X_2	2	2	−2	−2	−2	2	0	0	0	0	0	0	0	0
X_3	2	−2	0	−2	2	0	0	0	0	0	0	0	0	0
X_4	2	−2	0	−2	2	0	0	0	0	0	0	0	0	0

TABLE V. Repeated operations of the space group for the four-site cluster in the square lattice and their identification with point-group operations. The cluster-permutation group is isomorphic to the point group C_{4v} with an origin at the center of the square. The space-group operations are denoted in the standard notation of a point-group operation followed by a translation all enclosed in curly braces. Put in more mathematical terms, this table explicitly lists the homomorphism that maps the space group onto the cluster-permutation group. The first row (corresponding to the redundant operations of the space group) forms the kernel of the homomorphism.

Point-group operation	Space-group operations		
E	$\{E\|0\}$,	$\{C_4^2\|0\}$,	$\{\sigma\|0\}$
C_4^2	$\{E\|\theta\}$,	$\{C_4^2\|\theta\}$,	$\{\sigma\|\theta\}$
C_4	$\{C_4\|\tau\}$,	$\{\sigma'\|\tau\}$	
σ	$\{E\|\tau\}$,	$\{C_4^2\|\tau\}$,	$\{\sigma\|\tau\}$
σ'	$\{C_4\|0,\theta\}$,	$\{\sigma'\|0,\theta\}$	

i.e., they are identical to the identity operation $\{E|0\}$, because the four-site cluster is self-contained. This implies that only irreducible representations of the space group that represent the twofold rotation and the reflections about the x and y axes by the unit matrix are acceptable representations.

The character table of the full space group (with the acceptable representations highlighted in bold) is recorded in Table IV. The cluster-permutation group, with all repeated operations eliminated, is isomorphic to the point group C_{4v} with its origin the center of the square. Table V shows the mapping between the space-group notation and the point-group notation for the group elements. The acceptable space-group representations can now be identified with the more traditional point-group representations: $\Gamma_1 \rightarrow A_1$, $\Gamma_3 \rightarrow A_2$, $M_1 \rightarrow B_1$, $M_3 \rightarrow B_2$, and $X_1 \rightarrow E$.

The eight-site sq lattice cluster [Fig. 1(b)] is in the high-symmetry regime. The subgroup H of the cluster-permutation group G is the full space group, containing 64 elements distributed among 16 classes. The Brillouin zone[15] is sampled at four symmetry stars: Γ $(d=1)$, M $(d=1)$, X $(d=2)$, and Σ $(d=4)$. The character table of H may be found in Table XVI of Ref. 8.

The 8-site sq lattice cluster is not a 1NN-determined lattice: If site 3 is placed arbitrarily on the lattice and its 1NN's (sites 2, 4, 6, and 8) are added, there are two inequivalent possibilities for the placement of the 2NN pair (sites 1 and 5). The permutation operator P that interchanges site 1 with site 5 will map the lattice (nonrigidly) onto itself, preserving the entire neighbor structure of the lattice. The cluster-permutation group G is then generated from the space group H by closure. The existence of this nontrivial permutation operator is a *finite-size effect* of the eight-site cluster with PBC since it occurs because the lattice is not a 1NN-determined lattice.

The cluster-permutation group is composed of 128 elements divided into 20 classes and recorded in Table VI. Note that the presence of the permutation operator P forces physically different space-group operations(such as the translations, rotations, and reflections) to be sometimes in the same class. In fact, four pairs of classes of H combine to form single classes of G (see Table VI): $\{E|\tau\}$

TABLE VI. Class structure and group elements of the 128-element cluster-permutation group of the eight-site square lattice cluster. The notation is the same as that of Table IV and Ω denotes the third-nearest-neighbor translation. The element P corresponds to the transposition of sites 1 and 5 [see Fig. 1(b)].

Class	Group elements			Size of class
1	$\{E\|0\}$			1
2	$\{C_4\|0,\theta,\Omega\}$			8
3	$\{C_4^2\|0,\Omega\}$			2
4	$\{\sigma\|0,\Omega\}$			4
5	$\{\sigma'\|0,\theta_\parallel\}$			4
6	$\{E\|\tau\}$,	$\{\sigma\|\tau_\perp\}$		8
7	$\{C_4\|\tau\}$,	$\{\sigma'\|\tau\}$		16
8	$\{C_4^2\|\tau\}$,	$\{\sigma\|\tau_\parallel\}$		8
9	$\{E\|\theta\}$,	$\{C_4^2\|\theta\}$		4
10	$\{\sigma\|\theta\}$			4
11	$\{\sigma'\|\theta_\perp,\Omega\}$			4
12	$\{E\|\Omega\}$			1
13	$P\{E\|0\}$,	$P\{C_4^2\|\Omega\}$,	$P\{\sigma\|\Omega\}$	4
14	$P\{C_4\|0\}$,	$P\{\sigma'\|\theta_\perp\}$		4
15	$P\{C_4^2\|0\}$,	$P\{\sigma\|0\}$,	$P\{E\|\Omega\}$	4
16	$P\{\sigma'\|0,\Omega\}$,	$P\{C_4\|\theta\}$		8
17	$P\{E\|\tau\}$,	$P\{C_4^2\|\tau\}$,	$P\{\sigma\|\tau\}$	16
18	$P\{C_4\|\tau\}$,	$P\{\sigma'\|\tau\}$		16
19	$P\{E\|\theta\}$,	$P\{C_4^2\|\theta\}$,	$P\{\sigma\|\theta\}$	8
20	$P\{C_4\|\Omega\}$,	$P\{\sigma'\|\theta_\parallel\}$		4

TABLE VII. Character table of the 128-element cluster-permutation group for the eight-site square lattice cluster. The class structure and group elements are given in Table VI. The classes are labeled by their number to save space in the table below. The last column gives the compatibility relations with the irreducible representations of the space group H (Table XVI of Ref. 8). The subscripts p, z, and n denote representations that have a positive character, zero character, or negative character, respectively, for the element $P\{E|0\}$. The symbol ϕ is used to denote representations that mix different wave vectors.

	1	8	2	4	4	8	16	8	4	4	4	1	4	4	4	8	16	16	8	4	
	c_1	c_2	c_3	c_4	c_5	c_6	c_7	c_8	c_9	c_{10}	c_{11}	c_{12}	c_{13}	c_{14}	c_{15}	c_{16}	c_{17}	c_{18}	c_{19}	c_{20}	
Γ_{1p}	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	Γ_1
Γ_{1n}	1	1	1	1	1	1	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1	Γ_1
Γ_{3p}	1	−1	1	1	−1	1	−1	1	1	1	−1	1	1	−1	1	−1	1	−1	1	−1	Γ_3
Γ_{3n}	1	−1	1	1	−1	1	−1	1	1	1	−1	1	−1	1	−1	1	−1	1	−1	1	Γ_3
M_{1p}	1	1	1	1	1	−1	−1	−1	1	1	1	1	1	1	1	1	−1	−1	1	1	M_1
M_{1n}	1	1	1	1	1	−1	−1	−1	1	1	1	1	−1	−1	−1	−1	1	1	−1	−1	M_1
M_{3p}	1	−1	1	1	−1	−1	1	−1	1	1	−1	1	1	−1	1	−1	−1	1	1	−1	M_3
M_{3n}	1	−1	1	1	−1	−1	1	−1	1	1	−1	1	−1	1	−1	1	1	−1	−1	1	M_3
ϕ_1	2	2	2	−2	−2	0	0	0	2	−2	−2	2	0	0	0	0	0	0	0	0	$\Gamma_2 \oplus M_2$
ϕ_2	2	−2	2	−2	2	0	0	0	2	−2	2	2	0	0	0	0	0	0	0	0	$\Gamma_4 \oplus M_4$
X_{1p}	2	0	2	2	0	0	0	0	−2	−2	0	2	2	0	2	0	0	0	−2	0	X_1
X_{1n}	2	0	2	2	0	0	0	0	−2	−2	0	2	−2	0	−2	0	0	0	2	0	X_1
X_{2z}	2	0	2	−2	0	0	0	0	−2	2	0	2	0	2	0	−2	0	0	0	2	X_2
$X_{2z'}$	2	0	2	−2	0	0	0	0	−2	2	0	2	0	−2	0	2	0	0	0	−2	X_2
ϕ_3	4	0	−4	0	0	2	0	−2	0	0	0	4	0	0	0	0	0	0	0	0	$\Gamma_5 \oplus X_3$
ϕ_4	4	0	−4	0	0	−2	0	2	0	0	0	4	0	0	0	0	0	0	0	0	$M_5 \oplus X_4$
Σ_{1p}	4	0	0	0	2	0	0	0	0	0	−2	−4	2	−2	−2	0	0	0	0	2	Σ_1
Σ_{1n}	4	0	0	0	2	0	0	0	0	0	−2	−4	−2	2	2	0	0	0	0	−2	Σ_1
Σ_{2p}	4	0	0	0	−2	0	0	0	0	0	2	−4	2	2	−2	0	0	0	0	−2	Σ_2
Σ_{2n}	4	0	0	0	−2	0	0	0	0	0	2	−4	−2	−2	2	0	0	0	0	2	Σ_2

and $\{\sigma|\tau_\perp\}$, $\{C_4|\tau\}$ and $\{\sigma'|\tau\}$, $\{C_4^2|\tau\}$ and $\{\sigma|\tau_\parallel\}$, and $\{E|\theta\}$ and $\{C_4^2|\theta\}$. The translation subgroup is no longer an invariant subgroup and eight irreducible representations of H (Γ_2, Γ_4, Γ_5, M_2, M_4, M_5, X_3, and X_4) must combine to form higher-dimensional representations of G. The character table is reproduced in Table VII and includes the compatibility relations between representations of the cluster-permutation group G and the space-group representations (of H) in the last column.

The case when the Hamiltonian contains only 1NN interactions has an enlarged symmetry group since the eight-site sq lattice cluster with 1NN-only interactions is identical to a bcc-lattice cluster with 1NN-only interactions[8] (see Sec. IV).

The 16-site sq lattice cluster [Fig. 1(c)] is in the lattice regime for arbitrary interactions. There is no extra symmetry beyond the space-group symmetry and further analysis proceeds in a standard fashion [the Brillouin zone[15] is sampled at six symmetry stars: Γ ($d=1$), M ($d=1$), X ($d=2$), Σ ($d=4$), Δ ($d=4$), and Z ($d=4$)]. Hidden symmetry exists when the Hamiltonian is restricted to 1NN interactions only. The cluster-permutation group then contains 384 elements divided into 20 classes. The nonrigid permutation operator that generates the cluster-permutation group from the space group is given in the Appendix. This group is identical to the point group of a four-dimensional hypercube[12] but will not be pursued further here.

IV. EXAMPLE: EIGHT-SITE CLUSTERS AND THE t-t'-J MODEL

As a further illustration, the eight-site clusters are examined in more detail. The sc lattice cluster is a self-contained cluster (see Fig. 1 of Ref. 8). The point-group operations (with origin at a lattice site) corresponding to a rotation by 180° about the x, y, or z axis, $\{C_4^2|0\}$, and the inversion $\{J|0\}$ are all redundant operations; i.e., they are identical to the identity operation $\{E|0\}$. Therefore, only irreducible representations of the space group that represent $\{C_4^2|0\}$ and $\{J|0\}$ by the unit matrix are acceptable representations. This is summarized in the character table for the cluster-permutation group (see Table XIII in Ref. 8). The cluster-permutation group is isomorphic to the full cubic point group, O_h, with an origin at the center of the cube defined by the eight sides of the cluster.

The bcc, fcc, and sq lattice clusters are all in the high-symmetry regime. The bcc lattice is constructed from two four-site sublattices. The points in the bcc Brillouin zone[15] sampled here are Γ, H, and N. The cluster-permutation group includes any independent permutation of the elements within each sublattice and the interchange of the two sublattices. The subgroup H corresponds to all translations and proper rotations and contains the following 14 representations (with corresponding dimensions in parentheses): Γ_1 (1), Γ_2 (1), Γ_{12} (2), Γ'_{15} (3), Γ'_{25} (3), H_1 (1), H_2 (1), H_{12} (2), H'_{15} (3), H'_{25} (3), N_1 (6), N_2 (6), N_3 (6), and N_4 (6). The character table is given in Table XIV of Ref. 8. The classes $\{E|\tau\}$ and $\{C_2|\tau_\perp\}$ combine to form one class of the cluster-permutation group as do the two classes $\{E|\theta\}$ and $\{C_4^2|\theta_\perp\}$ and the three classes $\{C_4|\tau\}$, $\{C_4^2|\tau\}$, and $\{C_2|\tau_\angle\}$. The only representations that are not required to stick together are then Γ_1, H_1, N_1, and N_4. The cluster-permutation group has 20 irreducible representations that satisfy the compatibility relations with H given in Table VIII.

The fcc lattice cluster-permutation group[16] has a subgroup H that corresponds to all translations and proper rotations (see Table XV of Ref. 8) and is generated by the space-group generators and the permutation operator P that transposes the origin with its 2NN. There are 20 irreducible representations as recorded in Table VIII.

The sq lattice cluster-permutation group has been studied in detail in Sec. III. The compatibility relations of the 20 irreducible representations can be found in the last column of the character table (Table VII). Note that in the case of 1NN-only interactions the eight-site sq lattice cluster is identical to the eight-site bcc lattice cluster.[8]

As an application of these enlarged symmetry groups, a model of strong electron correlation (the t-t'-J model) is studied on these eight-site clusters. The t-t'-J model involves hopping between 1NN and between 2NN (excluding any double-occupation of a site) and a Heisenberg antiferromagnetic 1NN exchange interaction. Previous work on this model[8] utilized only the symmetry of the subgroup H of the space group. Use of the cluster-permutation group simplifies the problem even further and explains most of the "accidental" degeneracies ob-

TABLE VIII. Reduction of the 20-irreducible representations of the cluster-permutation group to the corresponding irreducible representations of the subgroup H of the space group for the body-centered- and face-centered-cubic lattice clusters. The dimensions of the irreducible representations of the cluster-permutation group label the columns.

	1	2	3	4	6	8	9	12	18
bcc lattice	Γ_1	$\Gamma_2\oplus H_2$		$\Gamma_{12}\oplus H_{12}$	N_1		$\Gamma'_{25}\oplus N_2$	$N_1\oplus N_4$	$\Gamma'_{15}\oplus H'_{15}\oplus N_2\oplus N_3$
	Γ_1			$\Gamma_{12}\oplus H_{12}$	N_1		$\Gamma'_{25}\oplus N_2$	$N_1\oplus N_4$	
	H_1			$\Gamma_1\oplus\Gamma_{12}\oplus H_2$	N_4		$H'_{25}\oplus N_3$		
	H_1			$\Gamma_2\oplus H_1\oplus H_{12}$	N_4		$H'_{25}\oplus N_3$		
fcc lattice	Γ_1	Γ_{12}	X_1	L_1	$\Gamma'_{15}\oplus X_4$	L_3			
	Γ_1	Γ_{12}	X_1	L_1	$\Gamma'_{25}\oplus X_3$	L_3			
	Γ_2		X_2	L_2	X_5				
	Γ_2		X_2	L_2	X_5				

TABLE IX. Symmetries of parameter-dependent eigenstates of the t-t'-J model that stick together in the eight-site clusters of the face-centered-cubic lattice and the square lattice. The sticking together of levels is *not* required by the cluster-permutation group. In the table below, N denotes the number of electrons and S denotes the total spin of the many-body wave functions. The subscript n denotes representations that have a negative character for the operation $P\{E|0\}$.

fcc lattice				sq lattice			
N	Symmetry	S	Number of levels	N	Symmetry	S	Number of levels
5	$L_{1n}\oplus L_{3n}$	$\frac{3}{2}$	2	4	$\phi_1\oplus\phi_3\oplus\phi_4$	2	2
5	$L_{1n}\oplus L_{3n}$	$\frac{1}{2}$	2	6	$\Gamma_{1n}\oplus M_{1n}$	2	2
6	$L_{1n}\oplus L_{3n}$	1	4	7	$\Gamma_{1n}\oplus M_{1n}$	$\frac{3}{2}$	2
7	$L_{1n}\oplus L_{3n}$	$\frac{3}{2}$	2				
7	$L_{1n}\oplus L_{3n}$	$\frac{1}{2}$	2				

served in the many-body energy levels. The largest Hamiltonian blocks that need to be diagonalized after the cluster-permutation group symmetry is incorporated are as follows: 5×5 for five electrons in the bcc lattice, 7×7 for six electrons in the fcc lattice, and 11×11 for six electrons in the sq lattice. It is interesting to note that, with the exception of two 5×5 blocks, the 6561×6561 Hamiltonian matrix can be diagonalized *analytically* for the bcc lattice.

There are only a few cases of extra degeneracies that remain in the energy spectrum. Most of these degeneracies involve parameter-independent eigenvectors; i.e., eigenvectors that do not depend on the hopping integrals t or t' or on the Heisenberg antiferromagnetic interaction J. The fcc and sq lattices both have *parameter-dependent* eigenstates with energy levels that stick together and are summarized in Table IX. This sticking-together[17] of levels would be explained if there was a larger symmetry group, an orbital-permutation group, that involves permutations mixing spatial and spin degrees of freedom, and contains the cluster-permutation group as a subgroup. The evidence in favor of this conjecture is that the extra degeneracies occur only between specific cluster-permutation group representations that have the same total spin.[18] A similar phenomenon was observed in the Hubbard model at half-filling on an eight-site sq lattice cluster.[13]

V. CONCLUSIONS

This contribution outlines the transition from a system that resembles an isolated cluster (point-group symmetry) to a system that resembles an infinite lattice (space-group symmetry). An intermediate region is discovered that has increased symmetry beyond that of the space group (it should be emphasized that *any* family of finite clusters that is used to approximate an infinite lattice will pass through this high-symmetry regime). These additional symmetry operations are nonrigid transformations that map the cluster into itself and form a group, the cluster-permutation group (which typically includes the space group as a subgroup). An analysis of the cluster-permutation group shows two different effects: (1) the Hamiltonian matrix for a given representation of the space group may split into irreducible blocks, and (2) irreducible representations of the space group (which frequently correspond to different points in the Brillouin zone) may "stick together." These two effects explain several puzzling degeneracies and level crossings found, numerically or analytically, in many cluster calculations.[8]

The order of the cluster-permutation group may be quite large (see for example the group of order 7 962 624 for the 16-site cluster in the fcc lattice). The extra symmetry of such a large group greatly facilitates the numerical problem of diagonalizing large Hamiltonians and may result in completely analytical solutions (as seen in the eight-site cluster in the fcc lattice).[18] The size of the cluster may be fairly large before this extra symmetry is lost (it survives up to the 64-site sc lattice cluster for Hamiltonians with 1NN interactions only). The effect of an enlarged symmetry group is more pronounced in systems with short-range-only interactions (compare Tables II and III) since many nonrigid transformations that map the cluster onto itself preserve only the 1NN structure of the lattice. 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 employed to reduce the Hamiltonian blocks or not.

The transition from the self-contained-cluster regime, through the hidden-symmetry regime, to the lattice regime were studied explicitly for the two-dimensional square lattice. The group theory for the eight-site clusters in the simple-, body-centered-, and face-centered-cubic lattices and in the square lattice were discussed in detail and applied to a model of strong electron correlation (the t-t'-J model). Most "accidental" degeneracies of the many-body energy levels are now explained. There is a strong indication that additional hidden symmetry remains in the fcc and sq lattices that mixes spatial and spin degrees of freedom.

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APPENDIX: LINEAR-PAIR RULE

A necessary (but not sufficient) condition for extra symmetry operations is the linear-pair rule: A linear pair is defined to be a pair of distinct opposite 1NN of a lattice site (i.e., the linear pair and the chosen lattice site all lie on a line). An infinite lattice has one unique lattice site that has both elements of the linear pair as 1NN. The linear-pair rule is satisfied whenever there is *more than one* lattice site that has both elements of the linear pair as 1NN. If the linear-pair rule is satisfied, then the cluster-permutation group may contain elements outside of the space group for Hamiltonians that include only 1NN interactions, but is a (proper or improper) subgroup of the space group otherwise.

The nonrigid permuation operations that can be constructed when the lattice satisfies the linear-pair rule involve a nonrigid transformation of the 1NN of a given site. If a permutation operation can be constructed that interchanges 1NN of a given site so that elements that initially formed a linear pair do not form a linear pair after the permutation, and this operation can be completed (consistently) to the entire cluster (preserving the 1NN structure of the lattice), then a nonrigid permutation operator has been discovered.

As an example, consider the 16-site sq lattice cluster [Fig. 1(c)]. The linear-pair rule is satisfied since both elements of the linear pair (2, 4) are 1NN to the sites 1 and 3. The permutation operator

$$\begin{bmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 & 13 & 14 & 15 & 16 \\ 11 & 12 & 13 & 14 & 3 & 4 & 5 & 6 & 7 & 8 & 1 & 2 & 15 & 16 & 9 & 10 \end{bmatrix}$$

is an order-6 element that corresponds to a nonrigid transformation of the sq lattice cluster onto itself preserving the 1NN structure of the lattice. It will generate the entire cluster-permutation group from the space group by closure.

The linear-pair rule is not a sufficient condition to produce extra symmetry for 1NN-only interactions since the 64-site bcc lattice and the 32- and 64-site fcc lattice clusters all satisfy the linear-pair rule, but do not have any additional symmetry beyond the space group (see Tables II and III).

It is interesting to note that the fcc lattice is the only lattice that has no extra symmetry for 1NN-only interactions (compare Tables II and III). This probably arises because the fcc lattice is not bipartite.[19]

[1]L. M. Falicov, *Group Theory and its Physical Applications* (University of Chicago Press, Chicago, 1966), pp. 144ff.

[2]J. Callaway, *Quantum Theory of the Solid State* (Academic, San Diego, 1974), Chap. 4.

[3]*Monte Carlo Methods in Quantum Problems,* Vol. 125 of *NATO Advanced Study Institute Series C,* edited by M. H. Kalos (Reidel, Dordrecht, The Netherlands, 1984).

[4]For a review, see L. M. Falicov, in *Recent Progress in Many-Body Theories,* edited by A. J. Kallio, E. Pajanne, and R. F. Bishop (Plenum, New York, 1988), Vol. 1, p. 275; J. Callaway, Physica B **149**, 17 (1988).

[5]Lattices are chosen that are compatible with the space group of the infinite lattice; i.e., the lattice is mapped onto itself by every element of the space group (not necessarily in a unique fashion). For example, a rectangular cluster with periodic boundary conditions would not be allowed as an approximation to a square lattice since a 90° rotation does not map the cluster onto itself.

[6]C. Kittel, *Quantum Theory of Solids* (Wiley, New York, 1987), pp. 179ff.

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[8]J. K. Freericks and L. M. Falicov, Phys. Rev. B **42**, 4960 (1990).

[9]There may be additional nonrigid operations that preserve only the 1NN structure of the lattice.

[10]An exception to the second possibility is the eight-site fcc lattice cluster. It is a 1NN-determined lattice, but the cluster-permutation group preserves the *entire* neighbor-structure of the lattice. The reason is each site has six sites that are 1NN and one site that is a 2NN. Therefore, any permutation operation that preserves the 1NN structure must, by default, also preserve the 2NN structure.

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[14]L. M. Falicov, *Group Theory and Its Physical Applications* (University of Chicago Press, Chicago, 1966), pp. 151ff.

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[16]J. K. Freericks and L. M. Falicov, Lett. Math. Phys. (to be published). This group has 384 elements, 20 classes and irreducible representations, and is also isomorphic to the point group of the four-dimensional hypercube.

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