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A Periodic Small-Cluster Approach to Many-Body Problems

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DISCLAIMER

A PERIODIC SMALL-CLUSTER APPROACH

TO MANY-BODY PROBLEMS

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INTRODUCTION

Many-body problems can very seldom be solved exactly, and their study normally requires approximate methods[1]. These approximations are of various kinds and accuracy, but usually they involve either a perturbation treatment, or a variational approach. The method employed also depends on whether the problem under study is a real or realistic system (e.g. the ferromagnetism of the surface of the ordered FeCo alloy[2]; the photoemission spectrum of nickel metal[3]; the thermal energy gap[4] of semiconducting Si) or a prototype, ideal model (e.g. the free-electron gas[1,5,6]; the one-dimensional Hubbard model[7,8]; the square-lattice Hubbard model[9]; the single-center Anderson impurity model[10,11]).

Perturbative treatments are based on previously determined one-particle states (which for realistic systems are only obtained, stored, and handled numerically), and diagrammatic inclusion of particle-interaction effects, based either on the Raleigh-Schrödinger or the Brillouin-Wigner perturbation scheme. The calculation of anyone of these diagrams involves in general a multidimensional integral in reciprocal space which, for periodic systems, extends in each variable over the reciprocal-space unit cell, the Brillouin Zone (BZ). These integrals are indeed very laborious and numerically intensive; by and large they are performed in a coarse way by sampling reciprocal space in very few points, in fact in no more points than time and computer memory would reasonably allow. Techniques for sampling the BZ have been developed[12]; they try to avoid the pitfall of choosing too regular a grid, which tends to select special points in the system. However, regardless of the technique, sampling in a set of N points in reciprocal space is always essentially equivalent to solving the problem in real space in a "minicrystal" of N sites with periodic boundary conditions[13].

The method proposed by the author and used with his collaborators in the solution of a variety of problems[14–23] consists of taking explicit advantage of this finite sampling $\leftrightarrow$ finite cluster duality. By a systematic, symmetric and wise choice of N points in reciprocal space, the problem can be reduced to that of a symmetric periodic cluster with N sites. If, in addition, N is small enough -- as is the case in the normal handling of perturbation expansions -- the problem can then be solved *exactly*, without recourse to perturbation methods. With the aid of group theory, only modest computer facilities are required. A similar approach has been taken by Callaway and his collaborators[24–26].

AN EXAMPLE: THE *fcc* LATTICE

Figure 1 shows a 32-atom portion of a face-centered cubic lattice, which is supposed to extend

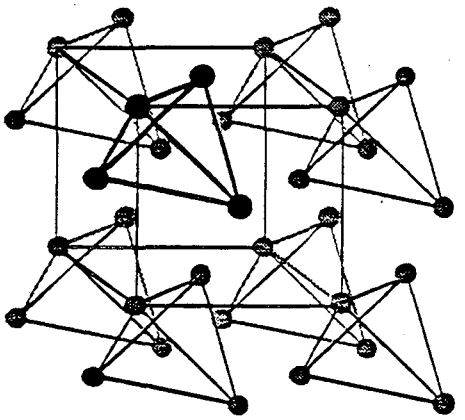

Fig. 1 Thirty-two-atom portion of the face-centered cubic lattice.

for an indefinite number of cells in all three directions and to satisfy periodic boundary conditions. Figure 2 shows the corresponding BZ, with some of its symmetry points indicated. If the crystal has N atoms, there are N allowed translations in the crystal. Since, in addition, the cubic group contains 48 point operations there are, all together, $48N$ symmetry space operations in the N-atom cluster system. It is now possible to select small clusters, preserving at all times the cubic symmetry of the crystal. The simplest cluster to choose is, of course, the single atom -- the Wigner-Seitz cell. The wavefunctions of that system have all the complete periodicity of the lattice, i.e. in the language of group theory they transform according to the Γ representations of the space group. Since Γ is the central point of the BZ (Fig. 2), a cluster of one atom is equivalent to sampling the BZ only at Γ. There are all together 48 group operations; they form the cubic point group O_h, and yield the set of the ten irreducible Γ representations [13,27].

A four-atom tetrahedral cluster is highlighted in Fig. 1. That small crystal has four internal translations and 192 symmetry operations. It should be emphasized that there are only four atoms in the crystal, in the sense that only four arbitrary phase factors for the wave functions can be chosen. The crystal structure, because of the periodic boundary conditions, is however still fully *fcc*, and each point preserves its complete *fcc* environment, e.g. each atom has twelve nearest neighbors, six second-nearest neighbors, etc. If the atoms within the tetrahedral cluster are labelled 0, 1, 2, and 3, the atom 0 has four nearest neighbors of type 1, four of type 2, and four of type 3; all six second-nearest neighbors atoms are of type 0. Wave functions such that all atoms of the same type have the same phase can only correspond to the four k-vectors labelled Γ and X, and shown in Fig. 2. A tetrahedral *fcc* cluster with periodic boundary conditions is equivalent to the finite sampling of the BZ at only the four points Γ and X. The group now consists of 192 operations and twenty irreducible representations; ten at Γ, ten at X.

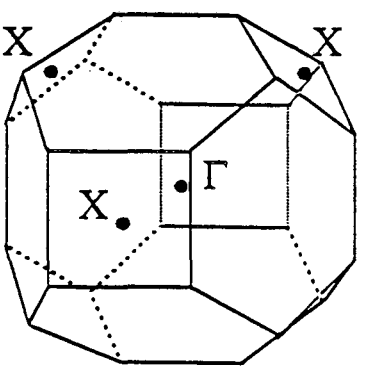

Fig. 2 The Brillouin Zone of the face-centered cubic lattice.

A larger cluster of eight atoms can be similarly constructed. It corresponds to doubling the original *fcc* unit cell, or -- even though not immediately obvious -- to choosing two adjacent tetrahedra in Fig. 1. If the atoms are labelled 0,...3 in the first tetrahedron, and similarly 4,...7 in the contiguous one, the twelve nearest neighbors of each atom 0 are two each of the types 1, 2, 3, 5, 6, and 7; all six second-nearest neighbors are of type 4. There are now 384 group operations. The corresponding eight-point sampling of the BZ includes the point Γ, the three points X, and the four points L (the centers of the hexagonal faces of the zone, not marked in Fig. 2). These twelve k-vectors yield 26 irreducible representations: ten at Γ, ten at X, six at L.

THE HUBBARD MODEL IN THE *fcc* LATTICE

Since its introduction in 1963, the Hubbard model[7] has become the prototype of a system of fermions with short-range interactions. It has been used to study a great variety of many-body effects in metals, of which ferromagnetism, antiferromagnetism, metal-insulator transitions, spin-density waves, charge-density waves, and superconductivity are the most common examples[7–9,16,22–26,28–33].

The model has been applied to a variety of lattices -- one, two, and three dimensional[8,22,28,29,34]. Exact solutions are available for one dimension[8], and exact theorems have been proved for some cases[35]. Since the numerical solution of extended cases is in general very laborious and computationally expensive[9,34], exact results easily obtainable with relatively small clusters with periodic boundary conditions[14–16,22,23] are an appealing alternative to study the model.

In a finite N-cluster with the N sites labeled $i = 0, 1, 2, N-1$, there is one s orbital per site, either spin up or down, denoted with subscript σ. The creation [destruction] operator is written as $c_{i\sigma}^{\dagger}$ [$c_{i\sigma}$]. The Hubbard Hamiltonian is:

$$H = - \sum_{\substack{i,j;\sigma \\ \textit{nearest neighbors}}} t\ c_{i\sigma}^{\dagger} c_{j\sigma} + \sum_{i} U\ c_{i\uparrow}^{\dagger} c_{i\uparrow} c_{i\downarrow}^{\dagger} c_{i\downarrow}.$$

The terms in H are: (1) a band "hopping" interaction between states on adjacent sites, with transfer integral t; (2) an on-site (intra-atomic) interaction U which can be either repulsive or attractive. The model, once the lattice is defined, is determined by (A) defining the cluster with N sites; (B) defining the dimensionless parameter [U/t]; (C) defining the sign of U; and (D) determining the number of particles n in the cluster, where $0 \le n \le 2N$, and [n/N], the number of particles per site, may vary between 0 and 2. The total number of available many-body states for each N-cluster is 2^{2N}, regardless of particle occupation. The number of many-body states for given N and n is [$(2N)! / n! (2N-n)!$]. Further major reductions in the secular equations to be solved can be achieved by means of group-theoretical methods, making use of the space-group and full spin-rotation symmetries.

Tetrahedral Cluster

The Hubbard model in the tetrahedral cluster[16] can be solved *analytically*, regardless of the number of particles n. The largest secular equation to diagonalize is of order 3. The results are interesting, and sometimes surprising:

(i) for n=2, t>0, the ground state of the system is always of symmetry $^1\Gamma_1$;

(ii) for n=3, t>0, the ground state of the system is always of symmetry $^2X_1$;

(iii) for n=4, t>0, U>0 the ground state of the system is of symmetry $^1\Gamma_{12}$, but a low-lying excited state of symmetry $^3X_2$ is always present; for U<0 the ground state of the system is of symmetry $^1\Gamma_1$, and a low-lying excited state of symmetry $^1X_1$ is always present;

(iv) for n=5, t>0, U>0 the ground state of the system is of symmetry $^4\Gamma_2$, and a low-lying excited state of symmetry $^2X_2$ is always present; for U<0 the ground state of the system is of symmetry $^2\Gamma_{12}$, and a very low-lying (almost throughout degenerate) excited state of symmetry $^2X_1$ is always present;

(v) for n=6, t>0, U>0 the ground state of the system is accidentally degenerate throughout, consisting of a state of symmetry $^1\Gamma_{12}$, and another of symmetry $^3X_2$; for U<0 the ground state is nondegenerate, of symmetry $^1\Gamma_1$, and a low-lying excited state of symmetry $^1X_1$ is always present;

(vi) for attractive interactions U<0, the ground states are always of minimum spin multiplicity;

(vii) for $t>0$ there are magnetic ground states for $n=5$ and 6, a feature that seems to be a consequence of the "piling up" of the one-electron states at the top of the band;

(viii) as U changes sign there are ground-state symmetry crossovers for $n = 4$, 5, and 6;

(ix) accidental degeneracies, a feature present in most Hubbard models, are once again present here;

(x) the piling-up of one-electron states at the top of the band -- and the lack of particle-hole symmetry in the model -- is a consequence of the triangular rings of the *fcc* structure, with its consequent "frustration" properties for states with alternating phases; this frustration is responsible for the richness of structure and the variety of states observed, as well as for the lack of validity of the Lieb and Mattis theorem[35];

(xi) if the tetrahedral cluster for $t>0$, $U>0$ is considered an "atom" and Hund's rules are applied to it, it can be observed that they are satisfied for $n = 0$, 1, 2, 3, 5, 7, and 8, violated for $n = 4$, and invalid (because of the accidental degeneracy) for $n = 6$.

Eight-Site Cluster with Seven Electrons

Because of the recent proposal by Anderson[26,33] that high-temperature superconductivity in complex Cu oxides could be interpreted in terms of an almost full, frustrated, Hubbard-type system with very large interactions (atomic or infinite-U limit), it is interesting to explore the (profoundly frustrated) *fcc* Hubbard model with occupation $[n/N]$ close to one. This has been accomplished[23] by using the eight-atom cluster, with an occupancy of $n = 7$, and in the limit $U \rightarrow +\infty$. In that limit there are 1024 seven-particle many-body states. These states contain either one or zero particle per site, form 69 symmetry-required energy levels, and are distributed among the various symmetries as shown in Table I.

TABLE I. Distribution of the 1024 States and 69 Energy Levels for the $N = 8$, $n = 7$, $U \rightarrow +\infty$, *fcc* Hubbard Model among the Various Symmetries[27].

	Γ_1	Γ_2	Γ_{12}	Γ_{15}'	Γ_{25}'	X_1	X_2	X_3	X_4	X_5	L_1	L_2	L_3
dim.	1	1	2	3	3	3	3	3	3	6	4	4	8
S=7/2	1	0	0	0	0	1	0	0	0	0	1	0	0
S=5/2	1	0	1	0	1	2	1	1	0	1	2	0	2
S=3/2	1	0	2	1	2	3	2	2	1	3	3	1	5
S=1/2	2	1	1	1	2	3	2	2	1	3	4	2	4

The results of these calculations are very illuminating. For $t<0$, when states "pile up" at the bottom of the band and the only available hole is near the well behaved, analytic top of the band, the ground state of the system is *ferromagnetic*, with symmetry ${}^8\Gamma_1$ and total cluster energy $-12|t|$. The inclusion of higher order terms, of order $[|t|^2/U]$, which make a relatively weak antiferromagnetic superexchange contribution, does not modify this result.

The $t>0$ case, on the other hand, is extremely complex. The "piling up" of states at the top of the band causes an extraordinary degeneracy of the many-body ground-state manifold, with 9 (out of 69) symmetry levels and 96 (out of 1024) states being all accidentally degenerate at the minimum cluster energy of $-6t$. Those nine symmetry levels are ${}^6X_2$, ${}^4\Gamma_{12}$, ${}^4X_1$, ${}^4X_2$, ${}^4L_2$, ${}^2\Gamma_2$, ${}^2X_1$, ${}^2X_2$, and ${}^2L_3$ -- i.e. spin sextets, quartets and doublets, as well as a variety of space symmetries. The inclusion or an antiferromagnetic interaction removes partly this degeneracy, but leaves 3 symmetry levels [${}^2\Gamma_2$, ${}^2X_1$, and ${}^2X_2$] and 14 states still degenerate in the ground-state manifold. The complexity of this manifold may allow extra splitting in the presence of other interactions (such as an electron-electron attractive interaction mediated by phonons), and thus serve as the basis for the competition between magnetic, metal-insulator and superconducting effects, which seem to be at the heart of high-temperature superconductivity.

THE PHOTOEMISSION SPECTRUM OF METALLIC NICKEL

Nickel metal has a very narrow one-electron d-band width (4.3 eV according to reliable band-structure calculations[36,37]) and a considerably strong intra-atomic electron-electron interaction, estimated to be[38] between 2.5 and 4.5 eV. It is therefore a very strongly correlated transition metal. Its photoemission spectrum[39–47] exhibits many interesting features and has been the subject of numerous theoretical contributions[3,17,48–53]. In particular three features require special attention, beacuse they cannot be explained based solely on one-electron, band structure effects:

(1) there are satellites in core-level photoemission spectra, approximately 6 eV below the main lines[39–41];

(2) resonant phtoemission was observed at 67 eV photon energies (the $3p \rightarrow 3d$ transition) for a satellite approximately 6 eV below the Fermi level[42–44];

(3) valence-band photoemission shows an apparent d-band width reduced by 25% and an exchange splitting reduced by 50% from the values obtained from band-structure calculations[45–47].

The problem is ideal for treatment by the small-cluster approach. It has thus been studied[17], in the four-atom tetrahedral approximation of the *fcc* lattice (the crystal structure of Ni metal), including ten electron orbitals per site, the one-electron energy parameters of Wang and Callaway[36], and full intra-atomic electron-electron interactions between the various d-orbital electrons. Atomic symmetry allows for three independent intra-atomic interaction parameters, normally labelled U, J, and ΔJ., which have been kept in the ratio 56:8:1, and scaled to provide the proper satellite spectral position. A value of U = 4.3 eV yields the best results.

The cluster consisting of 4 sites contains 40 d-orbitals; 38 electrons (2 holes) were included in the ground state, yielding an average occupancy of 9.5 d-electrons per atom, very close to the observed value[54] of 9.46. For two holes the tetrahedral cluster with the Hamiltonian described above yields an accidentally degenerate ground state of symmetries ${}^3X_2$, ${}^1\Gamma_2$, and ${}^1\Gamma_{12}$. If nearest neighbor exchange is included, the ferromagnetic ${}^3X_2$ state has the lowest energy. This state, obtained analytically, contains only holes in the X_5, minority-spin one-electron orbitals. Because of the Pauli exclusion principle it has zero probability of having two holes in one site: the holes are (through exchange) perfectly correlated with one another, and consequently, counting from the full d-shell, there is no contribution to the ground-state energy from the one-site, hole-hole interaction.

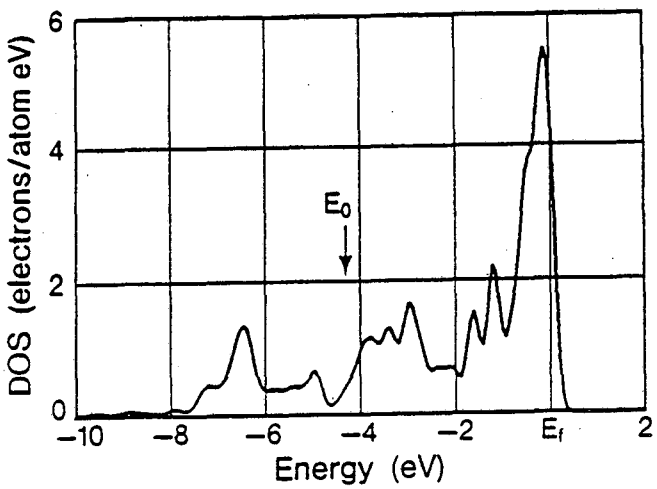

Fig. 3 The total density of calculated emitted one-electron states in metallic nickel. The location of the lowest single-electron state at X in the d-band according to Ref. 36 is denoted by E_0.

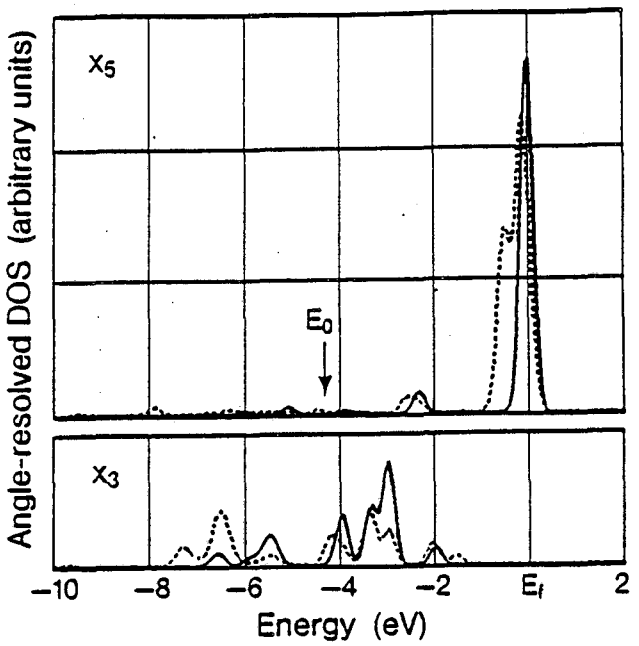

Fig. 4 Density of emitted states in metallic nickel, projected on the wave vector and symmetry of the emitted electron. Solid lines correspond to minority-spin states; dashed lines are for majority-spin states.

The photoemission process introduces a third hole into the system. The three-hole manifold of the tetrahedral cluster contains 9880 many-body states. The use of group theory simplifies the matrix considerably: the largest secular problem to solve, once group factorization has been accomplish, is of order 238. If final-state effects (such as variations in the density of the emitted-electron states, or resonance effects involving core electrons) are neglected, the observed, non-resonant density of photoemission states -- the photoemission spectrum -- is obtained by projecting the $^3X_2$-ground-state with an extra hole into the three-hole energy-eigenvalue spectrum. By selecting the desired one-electron-orbital k-vector, space and spin symmetries of the extra hole (the photoemitted electron), angular resolution (only for k-vectors at Γ and X), spin polarization and spatial distribution spectra can be determined.

Figure 3 shows angle-, symmetry- and spin-integrated results. The discrete spectrum of 9880 lines has been broadened with a narrow Gaussian of 0.15 eV half-width. It compares well with experiment not only in the existence of a satellite, but in its relative intensity with respect to the main band of the spectrum. Projected densities of emitted states with symmetries X_5 and X_3 for the photoelectron are shown in Fig. 4. States of X_5 symmetry, near the Fermi level, are characterized by single, narrow peaks. States of X_3 symmetry, near the bottom of the band, have strong satellite components and exhibit a well known multiplet structure.

The results yield the following conclusions:

(i) three-hole eigenstates corresponding to the "main band" have a greatly reduced probability of finding two holes in the same atom (20% at the Fermi level, 5% at the bottom of the band), as opposed to 50% in a random state created from the $^3X_2$ ground state;

(ii) three-hole eigenstates in the satellite part of the spectrum have a very high probability of finding two holes in one atom;

(iii) the many-body calculation yields a considerably reduced banwidth of 3.4 eV, in excellent agreement with the experimental value[45–47] of 3.3 eV, and considerably reduced from the band-structure[36] value of 4.3 eV;

(iv) band-structure calculations yield a Fermi-level X_5 line which consists only of majority-spin electrons -- the corresponding minority-spin states are above the Fermi level, i.e. empty; the results of Fig. 4 clearly point out that the X_5 Fermi-level line is a combination of both spins, that the minority X_5 states are appreciably occupied in the true many-body states, and that the exchange splitting of that X_5 level is very small;

(v) agreement with experimentally determined values of the spectral lines is very good throughout, with the exception -- similar to previous work[48] -- of the energy of the assigned X_2 symmetry.

CONCLUSION

In addition to the calculations reported here, the small-cluster approach has been successfully used to solve a variery of other problems: a periodic Anderson model to study thermodynamic and spectral properties of fluctuating-valence and heavy-fermion solids[18,19]; the ferromagnetic and photoemission properties of metallic iron[20] and the iron-cobalt ordered alloy[55]; the influence of many-electron effects on the ordering and segregation properties of binary and ternary alloys[21]; the itinerant and localization properties of hydrogen and deuterium on metallic surfaces[22] ; the possibility of phase transitions as a function of the parameters in the extended (additional intersite, nearest neighbor interaction) one-dimensional Hubbard model[34,56].

The method has the obvious advantage that it does not involve perturbation expansions, so the validity of its findings does not depend on "hoping" that the series employed converges for the properties under study. It is good for determining either uniform or short-range properties of periodic systems. In particular it is excellent for those short-range properties that are essentially atomic but are profoundly modified by the solid-state environment. The study of longer-range properties can be accomplished with larger clusters, but the complexity of the problem grows exponentially with the number of orbitals considered. Even with group-theoretical manipulations, moderate-size clusters can get out reach or control very easily. It is of course not a suitable approach to study long-wavelength phenomena, or interactions with long-range tails.

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