Exact Eigenvalues of the Constant-Coupled One-Band Model with a Finite Number of Sites

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The exact eigenvalues (for ground and excited states) of the constant-coupled one-band model for N_f fermions on N sites were obtained. Both electrons ($T<0$, where T is the coefficient of the term representing the "hopping energy") and holes ($T>0$) were considered, and results were obtained for $2 \leq N_f \leq N$ and $N=2$, 3, and 4. Only the $N_f=2$, $N=3$ and $N_f=3$, $N=4$ with $T>0$ cases gave a purely ferromagnetic ground state. These cases also showed a ferromagnetic state at higher energy. The eigenvalues were calculated as a function of U/T, where U represents the Coulomb energy of repulsion for electrons on the same site. The total spins of the states were obtained from their splitting in a magnetic field. The hopping term was found to be dominant for $|U/T|$ as large as one. The calculations support the suggestion that the ground state is usually antiferromagnetic.

I. INTRODUCTION

A model for certain aspects of magnetic behavior in transition metals is defined by the Hubbard Hamiltonian.[1-4] The model defined by this Hamiltonian can perhaps more accurately be called the short-range one-band model. The calculations to be described were done on a constant-coupled one-band model. However, for many of our small-finite-site calculations, every neighbor can be considered a nearest neighbor, and in this case there is no distinction between the two models. Thus many of our results have relevance for the Hubbard model and therefore should be of some physical interest. As a model for transition metals, the Hubbard Hamiltonian has serious defects; nevertheless, it has been the subject of considerable literature. A recent review article on the Hubbard Hamiltonian has been given by Khomskiy,[5] and Herring[6] has written a comprehensive review of the fundamental aspects of itinerant magnetic phenomena. The Hubbard Hamiltonian has also been related to the occurrence of insulating and metallic states in transition-metal oxides.[7]

A principal question concerning the Hubbard Hamiltonian is the nature of the ground state. It is not clear, for physically interesting cases, whether the exact ground state of the Hubbard Hamiltonian is ever ferromagnetic. Kemeny[8] has rigorously shown that a maximum-spin ferromagnetic state alone cannot be the ground state for systems which contain the same number of electrons as sites. For this case in the strong correlation limit, one can argue rather convincingly that the ground state is antiferromagnetic.[5] Lieb and Mattis[9] have ruled out a ferromagnetic ground state for a variety of nonphysically realistic systems. Their results are, however, applicable to the one-dimensional Hubbard Hamiltonian with nearest-neighbor (nn) coupling, for which Lieb and Wu[10] have obtained an exact ground-state solution. The state is antiferromagnetic with total spin zero for an even number of electrons. Nagaoka[11] has considered the variation of electron concentration and finds certain cases in which there is a ferromagnetic ground state. Nagaoka finds a ferromagnetic ground state for simple-cubic, face-centered-cubic, body-centered-cubic, and hexagonal close-packed structures when the number of electrons (N_e) is slightly greater than the number of sites (N), provided $|U/T|$ is sufficiently large. U represents the Coulomb energy of repulsion for electrons on the same site, and T is the coefficient of the term representing the hopping energy. Nagaoka's results have been extended somewhat by Sokoloff[12] who argues for their validity over a wider range of electron concentration. It should also be mentioned that many people believe that a ferromagnetic ground state can be induced if more degeneracy is allowed than in the narrow s-band Hubbard Hamiltonian, and if intra-atomic or Hund's rule coupling is included. A discussion of this point has been given by Van Vleck.[13]

It is well known that the Hubbard Hamiltonian with a large value of $|U/T|$ corresponds to a localized picture of magnetic moments, whereas a small value of $|U/T|$ corresponds to a very itinerant model. Inasmuch as the transition metals presumably are best characterized by an intermediate value of $|U/T|$, a study of the eigenvalues of the Hubbard Hamiltonian as a function of U/T is of some interest. Also, both excited and ground states are required for the calculation of the thermodynamic properties; therefore, all eigenvalues of the Hubbard Hamiltonian are of interest in gaining insight into the model's magnetic behavior as a function of temperature.[14]

The present paper attempts to understand the nature of the solutions of the Hubbard Hamiltonian

through the study of a finite number of electrons distributed over a finite number of equally coupled sites. Of interest is the effect of U/T and electron concentration in determining the nature of the states, with particular reference to the ground state. The use of a small finite number of sites and electrons makes it both possible and practical to obtain exact eigenvalues and eigenstates.

With completely straightforward computer programs, exact-energy eigenvalues as a function of (U/T) have been obtained for the 2 (= number of fermions N_f) on 2 (= N), 2 on 3, 2 on 4, 2 on 5, 2 on 6, 3 on 3, 3 on 4, and 4 on 4 cases. Both the $T>0$ (holes) and $T<0$ cases have been considered. The total spin of each state was identified by examining the variation of the energy eigenvalues with magnetic field. In principle, our finite models could be solved exactly by analytical techniques. In practice, the computer provides, for most cases, a much more practical method of obtaining these exact solutions.

In Sec. II a few (well-known) properties of the constant-coupled one-band model that are relevant to our calculation are summarized. In Sec. III the method and results of our calculation are given. In Sec. IV the results are discussed and a few suggestions for further work are presented.

II. SOME PROPERTIES OF THE CONSTANT-COUPLED ONE-BAND MODEL

Our Hamiltonian in the Wannier representation can be written

$$H = T \sum_{\alpha,\alpha',\sigma}{}' C^{\dagger}_{\alpha\sigma} C_{\alpha'\sigma} + U \sum_{\alpha} n_{\alpha\uparrow} n_{\alpha\downarrow} - h \sum_{\alpha,\sigma} n_{\alpha\sigma}\sigma , \tag{1}$$

where the first term is the hopping energy, the second is the Coulomb potential energy, and the third is the Zeeman energy. The sites are labeled by α and the spin by σ. We assume $\sigma = \pm\frac{1}{2}$ for alignment ($\uparrow$) or antialignment ($\downarrow$) of the spins with the magnetic field h (assumed to be in suitable units). The creation and annihilation operators for a fermion on site α with spin σ are given by $C^{\dagger}_{\alpha\sigma}$ and $C_{\alpha\sigma}$. The corresponding occupation number operator is given by $n_{\alpha\sigma} = C^{\dagger}_{\alpha\sigma} C_{\alpha\sigma}$. As mentioned previously, T is a measure of the ease of hopping between sites, and U determines the Coulomb potential energy between electrons with opposite spins on the same site. The prime on the sum means to omit the $\alpha = \alpha'$ term.

A. Spin Angular Momentum

The z axis is chosen as the direction of the magnetic field. The components of spin associated with the site α can be written

$$\sigma_{\alpha z} = \tfrac{1}{2}(n_{\alpha\uparrow} - n_{\alpha\downarrow}) , \tag{2}$$

$$\sigma_{\alpha y} = -\tfrac{1}{2} i (C^{\dagger}_{\alpha\uparrow} C_{\alpha\downarrow} - C^{\dagger}_{\alpha\downarrow} C_{\alpha\uparrow}) , \tag{3}$$

$$\sigma_{\alpha x} = \tfrac{1}{2}(C^{\dagger}_{\alpha\uparrow} C_{\alpha\downarrow} + C^{\dagger}_{\alpha\downarrow} C_{\alpha\uparrow}) . \tag{4}$$

The total spin operator of our system can then be written

$$\vec{S} = \sum_{\alpha} \vec{\sigma}_{\alpha} . \tag{5}$$

$\vec{S}$ is a valid angular momentum operator because from its definition it can be shown to satisfy the appropriate commutation relations. One can also directly verify that $[H, S^2] = 0$ and $[H, S_z] = 0$, where H is defined by Eq. (1) and $\vec{S}$ is defined by Eq. (5). One can therefore construct eigenstates of the Hamiltonian that have definite total spin and definite z component of the total spin. Furthermore, matrix elements of the Hamiltonian between states that differ in total spin or total z component of spin must vanish.

B. Electron-Hole Symmetry

We follow the usual procedure and choose $T<0$ for electrons and $T>0$ for holes.[11,13] The sign of T is important because the nature of the ground state may depend on the sign. U is positive because it represents repulsive Coulomb interactions.

Although the electron-hole symmetry of the Hamiltonian is an elementary property, it will be briefly discussed for clarity. Consider Eq. (1) with N electrons on N sites. Inasmuch as creating an electron destroys a hole, we have $C^{h}_{\alpha,-\sigma} = C^{e\dagger}_{\alpha,\sigma}$, where the superscripts h and e refer to holes and electrons, respectively. Thus by the anticommutation relations for fermion creation and annihilation operators, we see that the kinetic energy for electrons is equal to minus the kinetic energy for holes. On the other hand, the Coulomb term $U\sum_{\alpha} n^{e}_{\alpha\uparrow} n^{e}_{\alpha\downarrow}$ converts to $U\sum_{\alpha} n^{h}_{\alpha\uparrow} n^{h}_{\alpha\downarrow} + U(N - N_h)$ for $N_h = 2N - N_e$ holes. At zero field, if

$$H_e = -|T| \sum_{\alpha,\alpha',\sigma}{}' C^{e\dagger}_{\alpha\sigma} C^{e}_{\alpha'\sigma} + U \sum_{\alpha} n_{\alpha\uparrow} n_{\alpha\downarrow} \tag{6}$$

is the Hamiltonian for N_e electrons on N sites, and if the Hamiltonian for $N_h = 2N - N_e$ holes on N sites is

$$H_h = +|T| \sum_{\alpha,\alpha',\sigma}{}' C^{h\dagger}_{\alpha\sigma} C^{h}_{\alpha'\sigma} + U\sum_{\alpha} n^{h}_{\alpha\uparrow} n^{h}_{\alpha\downarrow} , \tag{7}$$

then

$$H_h = H_e - U(N - N_h) , \tag{8}$$

which defines the relation between the energy spectrum for electrons and holes. Note that the spectrum for N electrons or N holes (on N sites) is the same.

C. Limits of Strong and Weak Interaction

In the extreme strong-interaction limit, T equals 0, and our Hamiltonian is easy to solve because it is diagonal in the Wannier representation. In the extreme weak-interaction limit, U equals 0 and the Hamiltonian can be diagonalized by use of the Bloch representation.[1] Basically, this technique has been used to find exact solutions for our finite models in this limit.

Fairly reasonable Hartree-Fock solutions can be obtained when $|U/T|$ is very small but not zero. However, these approximate solutions break the rotational symmetry of our Hamiltonian, and the concern here is with exact solutions. For large $|U/T|$, the Hubbard Hamiltonian (when $N_e = N$) can approximately be replaced by a Heisenberg Hamiltonian with antiferromagnetic coupling.[13] This replacement does, however, eliminate the highest energy states.

III. METHOD AND RESULTS OF CALCULATION

A straightforward method of calculation was used. Basis states in occupation-number space were chosen, the matrix elements of the Hamiltonian for these states were generated, and the resulting eigenvalues were computed as functions of U, T, and h. The basis states were chosen by specifying $n_{\alpha\sigma}$ (here used as occupation numbers rather than occupation-number operators) and so were of the form $n_{1\uparrow}, n_{1\downarrow}, n_{2\uparrow}, n_{2\downarrow}, \cdots$, where for N_f fermions $\sum_{\alpha,\sigma} n_{\alpha\sigma} = N_f$. For N sites the number M of N_f-particle basis states is given by

$$M = \frac{(2N)!}{(2N - N_f)!\,N_f!} \quad . \tag{9}$$

We can use an array $N(I, J)$ to specify all basis states. A particular state of the basis will be designated I, and J will refer to the subscripts that label the occupation number. Thus, for example, $J = 3$ will correspond to $2\uparrow$, and $N(I, 3)$ is the value of $n_{2\uparrow}$ in state I. $N(I, J)$ will be 0 or 1 for all values of I and J. From the known properties of the fermion creation and annihilation operators, an explicit expression for the matrix elements can be derived. We assume all distinct sites are equally coupled. The kinetic-energy operator T_{op} contributes only off-diagonal terms to the matrix elements. These matrix elements are

$$\langle I'|\,T_{op}\,|I''\rangle = T(1 - \delta_{I'}^{I''}) \times \sum_{J,J'} [(1 - \delta_J^{J'})\,\delta_{N(I'',J')}^{N(I',J')-1}\,\delta_{N(I'',J)}^{N(I',J)+1}\,\delta_{J-J'}^{0(\mathrm{mod}2)} \times (\prod_{J''(\neq J,J')} \delta_{N(I'',J'')}^{N(I',J'')})(-)^A] \quad , \tag{10}$$

where

$$A = \sum_{J_1=1}^{J'-1} N(I'', J_1) + \sum_{J_2=1}^{J-1} N(I', J_2) \quad .$$

I' and I'' both range from 1 to M and the sums and products over the J's range from 1 to $2N$. The Kronecker δ involving 0(mod2) constrains J and J' to differ by an even integer. Physically this takes into account that the hopping term does not flip the spin. The Coulomb energy and the Zeeman energy are diagonal in the Wannier representation. Thus the matrix elements of the Hamiltonian are given by

$$\langle I'|H|I''\rangle = \langle I'|\,T_{op}\,|I''\rangle + \delta_{I'}^{I''}\,U \sum_{J=1}^{2N} N(I', 2J-1) \times N(I', 2J) - \delta_{I'}^{I''}\,(h/2) \sum_{J=1}^{2N} [N(I', 2J-1) - N(I', 2J)] \quad . \tag{11}$$

In the computations, it is useful to realize that $\langle I'|H|I''\rangle = \langle I''|H|I'\rangle^*$.

When the number of fermions, the number of sites, and T, U, and h, were given, the computer was programmed to generate the basis states [the array $N(I, J)$], compute the matrix elements by Eqs. (10) and (11), and find the eigenvalues of the resulting matrix. The results of these computations are presented below.

The major information in our calculations is contained in Figs. 1–3, which are smooth curves of the energy eigenvalues (E) divided by T drawn through calculated points at $U/T = 0$, 0.5, 1.0, and 2.0 with $h = 0$. Note that the 3 on 4 "hole" case (Fig. 1) has a "ferromagnetic" ground state. By ferromagnetic we mean a maximum-spin ground state, and by "antiferromagnetic" a minimum-spin ground state. Additional calculations, whose results are presented in Table I, have been made. The type of ground state obtained is summarized in the table. From the additional calculations, only the 2 on 3 hole case showed a purely ferromagnetic ground state. Figures 1–3, which are for a four-site problem, can be considered to represent a regular tetrahedron of sites with nn coupling. Similarly, the three-site case can be considered as an equilateral triangle, and the two-site case as a dumbbell; both cases with nn coupling. In Table I, the five- and six-site cases are not particularly physically realistic because of the assumption of equal coupling of sites.

IV. DISCUSSION AND SUGGESTIONS FOR FURTHER WORK

For Figs. 1–3 we note that the energies of the states of maximum spin are independent of U/T. If the number of fermions is less than or equal to the number of sites, then, by the Pauli principle, maximum spin is obtained when all fermions are on different sites. If the fermions are never on

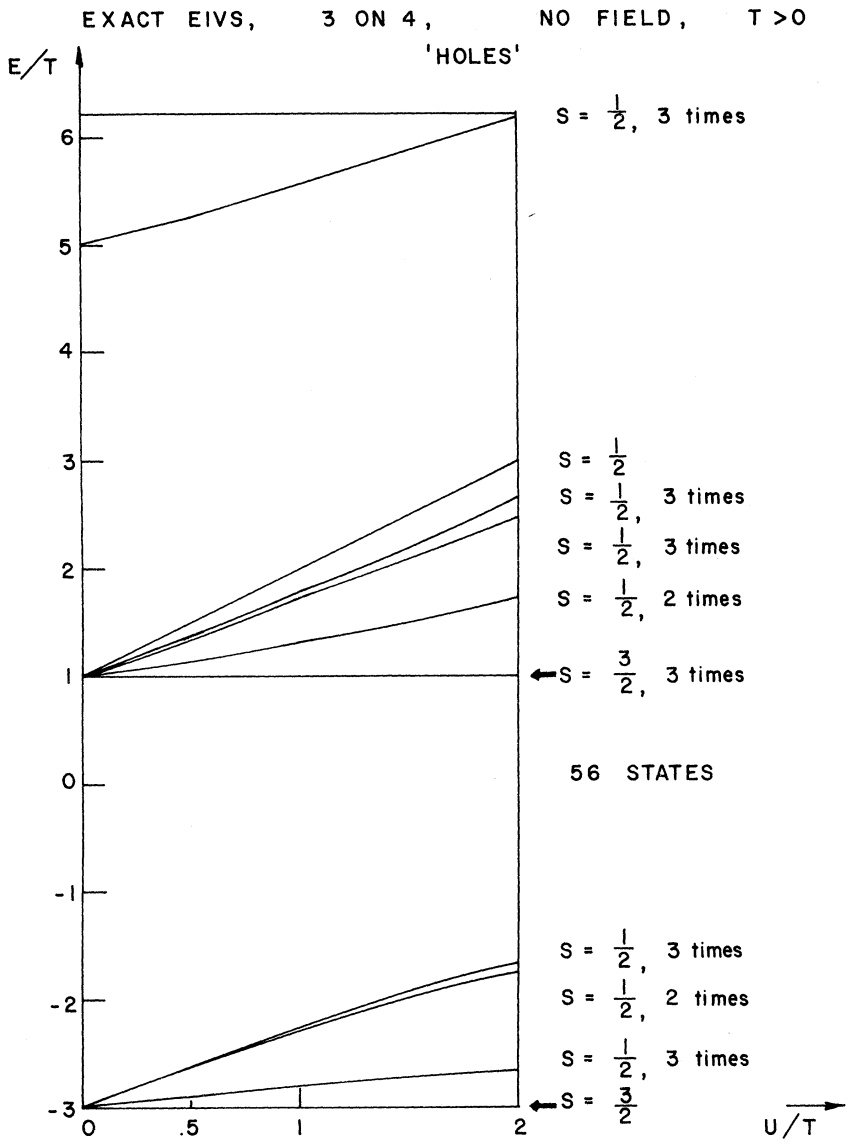

FIG. 1. The 56 energy eigenvalues (EIVS), E for 3 holes on 4 sites as a function of the ratio of Coulomb to hopping coefficients (U/T) with $h=0$.

the same site, they do not experience the Coulomb repulsion and so their energy is independent of U. Also, all calculations show a low spin value associated with the highest energy state, which might be expected from the association of high energy with double occupancy of sites.

As mentioned, Nagaoka[11] has predicted that if N_e is greater than and nearly equal to N (or N_h is less than and nearly equal to N), and if the Coulomb energy is sufficiently strong, then the Hubbard model for several crystal lattices should have a ferromagnetic ground state. Although the model for Fig. 1 corresponds to Nagaoka's conditions only by analogy, the occurrence of a ferromagnetic ground state might have been deduced by pursuit of this analogy. Similar considerations would lead one to expect that the model of Fig. 2 would not have a ferromagnetic ground state. Our results agree with this expectation. As can be seen from Table I, our calculations do lend support to the concept that the ground state of our Hamiltonian is a purely ferromagnetic state only for special conditions.

In Fig. 1 the highest spin value occurs both at the lowest energy and at a higher energy. For completely localized spins, if the lowest state is ferromagnetic, the higher states can be considered to have more spin disorder. Thus, if the spins are allowed the extra freedom of hopping, qualitative differences in the distribution of energy levels are produced. The occurrence of a maximum spin value at two different energies is also seen in Fig. 2.

If $U=0$, the energy spectrum of N_e electrons

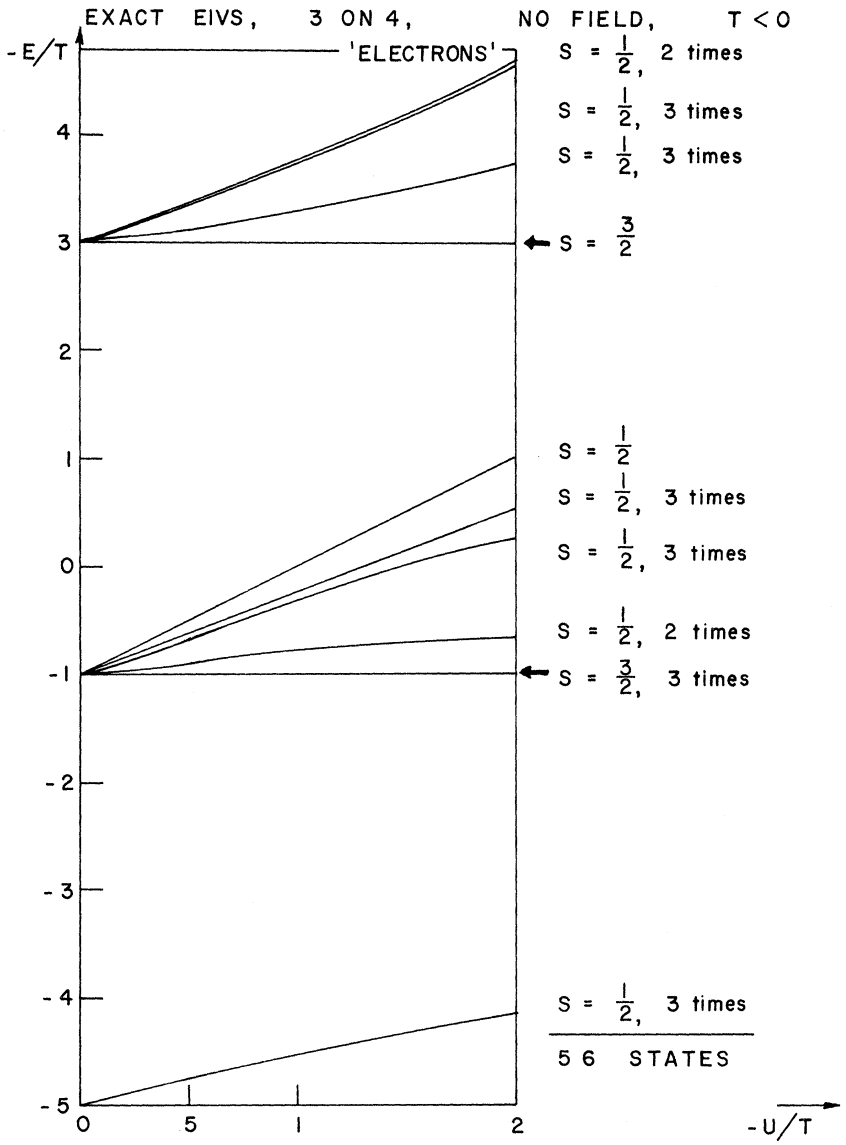

FIG. 2. E/T vs U/T with $h=0$ for 3 electrons on 4 sites. E = EIVS = eigenvalues.

($T<0$) is the negative of the energy spectrum of $N_h=N_e$ holes ($T>0$). Thus the total spread of the energy spectrum for both cases is the same, as shown in Figs. 1 and 2. However, even for $U\neq 0$, the spread in energies in Figs. 1 and 2 is about the same.

In Fig. 3, just above the antiferromagnetic ground state, a nonzero nonmaximum spin state exists. This combination could lead to unusual thermodynamic properties. For example, a magnetic field would lower one sublevel of the nonzero spin state to an energy below the ground state. Therefore, at low temperatures, this system should show a large change in the magnetic susceptibility as a function of field. Figure 3, for the 4 on 4 case is consistent with Kemeny's theorem[8] that N fermions on N sites do not have a purely ferromagnetic ground state. The fact that the ground state is antiferromagnetic in this case supports nonrigorous arguments[5,13] presented for large $|U/T|$. Antiferromagnetic ground states were obtained for the 3 on 3 and 2 on 2 cases as would be expected.[9,10]

In Figs. 1–3 for $|U/T|\leq 1$, the energy levels all tend to be in one of three distinct groups. The exact solution at $U=0$ shows that the grouping is a hopping energy effect. As mentioned, the $U=0$ solution can be obtained fairly easily by analytical techniques, and we find that the splitting into exactly three groups is a consequence of assuming all sites are equally coupled.

With $h=T=0$ the allowed energies are integral multiples of U. Thus for the 2 on 2 case, the energies would be 0 and U; for the 4 on 4 case the

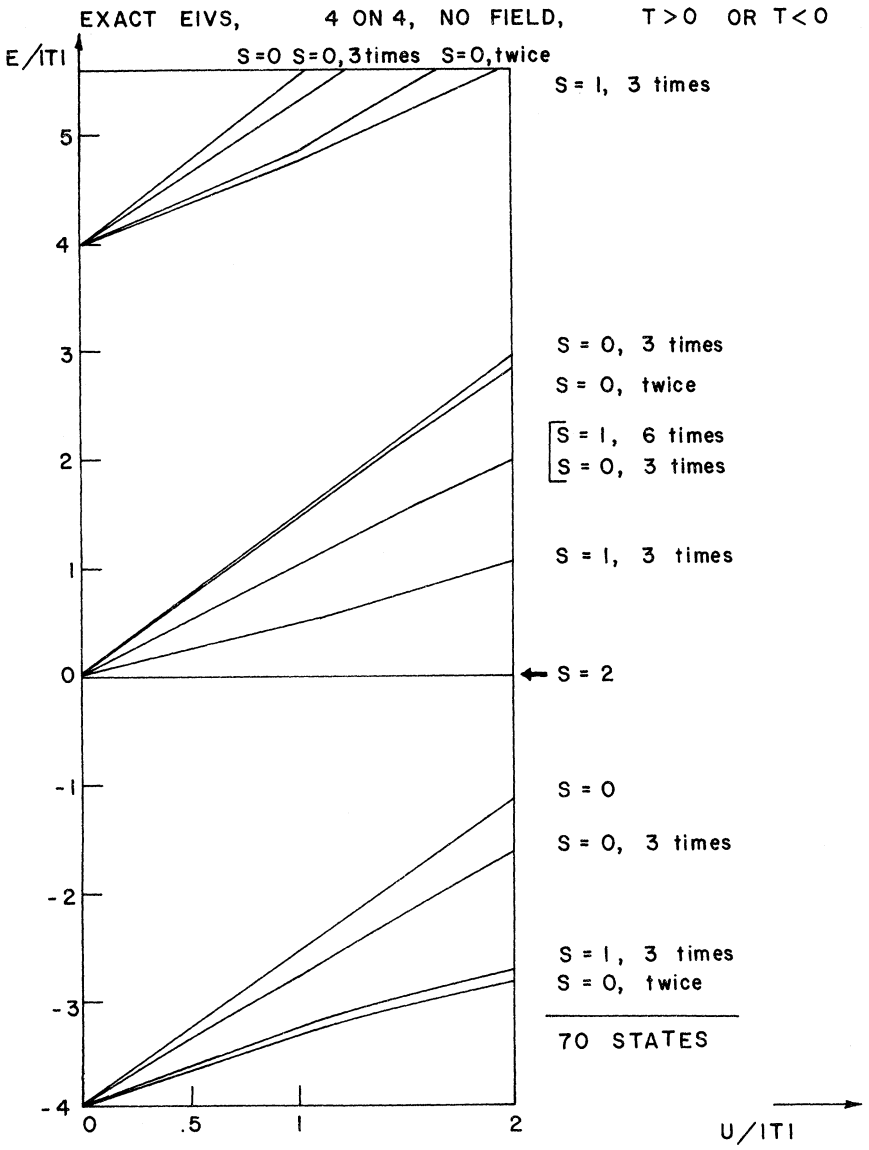

FIG. 3. E/T vs U/T with $h=0$ for 4 electrons on 4 sites. This case involves 70 eigenvalues (EIVS).

energies would be 0, U, and $2U$. The range of U/T in Fig. 3 is too small to see this trend; however, an actual calculation with $U/T=100$ showed a strong bunching of levels about $E/T=0$, 100, and 200. Only the $E/T=100$ level showed any appreciable spread, and it was on the order of ± 3. As might be expected, the 2 on 4 case (both signs of T) showed less variation in the energies as a result of increasing U than did the 4 on 4 case. The fermions in this case can more easily avoid double occupancy of sites. For the N on N case, the ferromagnetic state is expected to be degenerate with the ground state as $U/T \to \infty$, because the ferromagnetic state will have energy zero (no hopping and no double occupancy), and, when $T=0$ (and $h=0$), the lowest eigenvalue of the Hamiltonian is zero. This trend was clearly noted for the 4 on 4 case with $U/T=100$.

For $T<0$, the 2 on N calculations showed a steady decrease of the ground-state energy as the number of sites N was increased. For $T>0$, the 2 on N calculations with $N \geq 3$ had a constant ground-state energy of $-2T$ corresponding to a ferromagnetic ground state (degenerate with an antiferromagnetic state for the $N=4$, 5, and 6 cases).

To date, firm conclusions for actual physical systems cannot be drawn from this type of work. We need to know the relation between the Hubbard Hamiltonian and actual physical systems, and how large to make our finite models so that they will accurately reflect the behavior of a given property of an infinite-site model. To answer the latter question, larger arrays may be considered and the

TABLE I. Nature of ground state of finite-site constant-coupled one-band model.

Number of particles	Number of sites	Sign of T	Type of ground state[a]	Number of times occurs
2	2	±	AF, $S=0$	1
2	3	+	F, $S=1$	1
2	3	−	AF, $S=0$	1
2	4	+	F, $S=1$	3
			AF, $S=0$	2
2	4	−	AF, $S=0$	1
2	5	+	F, $S=1$	6
			AF, $S=0$	5
2	5	−	AF, $S=0$	1
2	6	+	F, $S=1$	10
			AF, $S=0$	9
2	6	−	AF, $S=0$	1
3	3	±	AF, $S=\frac{1}{2}$	2
3	4	+	F, $S=\frac{3}{2}$	1
3	4	−	AF, $S=\frac{1}{2}$	3
4	4	±	AF, $S=0$	2

[a]F means ferromagnetic, and AF means antiferromagnetic. The calculations were, for the most part, for $|U/T| \leq 2$, but some calculations outside this range suggest that the results in this table are probably valid for $0 < |U/T| < \infty$.

assumption that all sites are equally coupled should be relaxed. In principle, one could calculate the eigenvalues of fairly large arrays by choosing a set of basis functions that arrange the matrix of the Hamiltonian in block diagonal form. This could be accomplished by construction of basis functions that are eigenfunctions of S^2 and S_z and are basis functions for the irreducible representations of the spatial symmetry group of the Hamiltonian. However, for practical calculations, the size of the arrays is still drastically limited.[14]

Other studies can usefully be made. From the exact energy levels, one can evaluate the partition function and hence derive all thermodynamic quantities. To date, this has been performed only for one dimension with nn coupling.[14] It might also be useful to consider, for finite models, the effect of generalization of the Hamiltonian to include degeneracy and Hund's rule coupling.[13]

The present results may be used as a guide to check approximation procedures that may be used later on systems of realistic size. Unfortunately, an approximation procedure might give good results on a finite system and fail on an infinite system, or vice versa. Nevertheless, the comparison of approximations and exact results on finite systems should aid in a physical understanding of the approximations.

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