Ferromagnetic Spin Excitations in a One-Band Metallic Loop

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A one-band periodic loop of N electrons on N sites interact by a two-body spin-independent potential, the band and the potential restricted so that only nearest-neighbor Wannier integrals occur, but otherwise arbitrary. The elementary excitations relative to the saturated ferromagnetic eigenstate are then found rigorously. The nature of the excitations and the condition for the stability of the ferromagnetic eigenstate are discussed. The excitations divide into continuum states, bound electron-hole (exciton) states below the band, and spin-wave states. The entire energy spectrum and the electron-hole correlation functions for the bound states are given. It is also shown that under certain conditions, the lowest-energy eigenstate among all one-spin-flip states has $S=\frac{1}{2}N$ and $M=\frac{1}{2}N-1$, where S is the total spin and M the z component of spin quantum numbers. This result offers, therefore, a possible violation of the Lieb-Mattis theorem in the subspace of one-band functions for a loop.

1. INTRODUCTION

THE purpose of the present paper is to solve exactly for the lowest excited states of a one-dimensional one-band ferromagnetic metal containing the complete two-body spin-independent interaction between nearest-neighbor Wannier sites. In a following paper the method is extended to three dimensions, but the major results are already apparent in one dimension.

The problem here is very similar to the one posed by Slater in 1937,[1] and solved there by perturbation theory. He approached the situation from two different limits and inferred from this that the general excitation spectrum would contain a band of continuum states plus some split-off states resembling collective motion. The exact nature of the splitting off was not considered in detail, and his main interest in the solutions was in the lowest spin-wave state, from which he obtained his criterion for a ferromagnetic ground state.

In the present paper, we solve the problem exactly for nearest-neighbor interactions and show in detail how the split-off branches occur, their characteristics, and that for nearest-neighbor interactions there are at most 3 such, one of which is a spin wave, the others very much like excitons. (For next-nearest-neighbor interactions, there would be at most 5, and so on.) In effect, the calculation of the present paper confirms almost all the qualitative features of the problem as originally suggested by Slater.

Of the many other articles in this field,[2] the one that seems to come closest to a general solution for the Coulomb interaction is by Paul.[3] He gave a general equation for the energy of the one-spin-flip state in terms of a set of $\frac{1}{2}N$ wave numbers, k_i, but there was no indication as to what combinations of the k's would give rise to what types of states. Solutions were obtained for a special choice of the k's, and under certain approximations, but we have found it very hard to compare his results with ours.

The calculation of this paper starts from the ferromagnetic eigenstate ($S=M=\frac{1}{2}N$) where S is the spin quantum number, M the z component of the spin quantum number, and N the number of sites in the loop. Our problem is worked for the number of electrons also equal to N. From the results of the paper, it will be seen that for certain values of certain parameters, U, V, J, etc., the lowest-energy state in the subspace for $M=\frac{1}{2}N-1$ (i.e., the elementary excitation spectrum) has $S=M+1$, rather than $S=M$. This then is a violation of the Lieb-Mattis (LM) theorem[4] which states that in a given M subspace the state of lowest energy must belong to $S=M$. Hence the ground state, according to the LM theorem, must belong to $S=0$, and cannot be ferromagnetic. Since our calculation is exact, and the LM theorem quite general, there would seem to be a contradiction.

It should be kept in mind, however, that we consider only a one-band subspace, whereas the LM theorem is

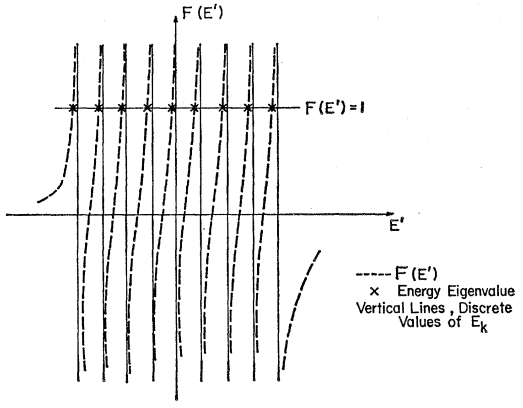

FIG. 1. This is a picture of Eq. (4.1). The intersections of $F(E')$, the dashed lines, with $F=1$ give the locations of energy eigenvalues.

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[1] J. C. Slater, Phys. Rev. **52**, 198 (1937).

[2] See, for example, E. D. Thompson, Ann. Phys. (N.Y.) **22**, 309 (1963); Y. Nagaoka, Phys. Rev. **147**, 392 (1966).

[3] D. Paul, Phys. Rev. **118**, 92 (1960).

[4] E. Lieb and D. Mattis, Phys. Rev. **125**, 164 (1962). See also D. Mattis, *Theory of Magnetism* (Harper and Row, Inc., New York, 1965).

general. Thus if the one-band model is *not* good, there is neither a contradiction with the LM theorem nor any significance to our results. But if there are situations where the one-band model *is* good, then there still is no contradiction with the LM theorem since we are forced to use periodic boundary conditions to solve the problem, whereas it is well known[5,6] that the argument leading to the LM theorem fails for periodic boundary conditions. For this reason, we suggest that the saturated ferromagnetic eigenstate can be a respectable candidate for the ground state of certain systems under certain potentials when interband effects can be neglected.

The Hamiltonian will be written in terms of Wannier functions $a(r-R_i)$ centered at the sites R_i. The band Hamiltonian (no interactions) is then written

$$H_b=\sum V_{ij}c_{i\sigma}{}^{\dagger}c_{j\sigma}, \tag{1.1}$$

where $c_{i\sigma}{}^{\dagger}$ is the creation operator, $c_{i\sigma}$ the destruction operator for an electron in the Wannier orbital i with spin σ, $\sigma=+,\ -$. The Wannier functions do not diagonalize the unperturbed Hamiltonian. They therefore have an energy spread, essentially the band spectrum.[7]

For narrow bands, Hubbard[8] has introduced a hierarchy of interaction terms the largest of which is

$$H_c=U\sum_i n_{i+}n_{i-} \tag{1.2}$$

representing the interaction of electrons of different spin at the same site.

The effect of the U term has been the subject of a great deal of work starting with Hubbard's original paper and culminating in Lieb and Wu's exact solution of the linear chain.[9] However, Slater already in 1937 had used this term in his fundamental paper on ferromagnetism,[1] and Slater, Koster, and Statz[10] in 1953 had used it to discuss the one-dimensional case of a band inhabited by two electrons.

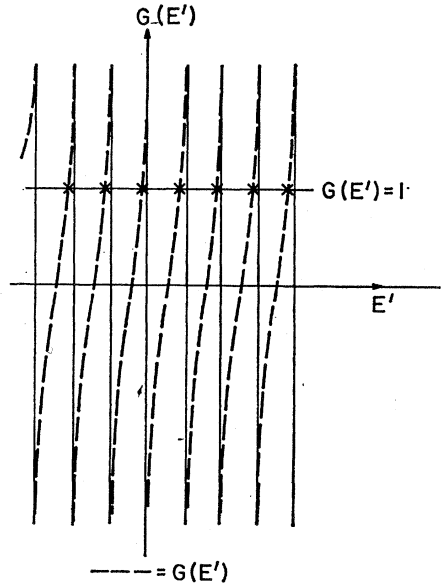

FIG. 2. This is a picture of Eq. (5.4) under the conditions in paragraph (1) below Eq. (5.8), in the continuum region.

Next on the list are the interactions between Wannier functions on two different sites, from which the follow-

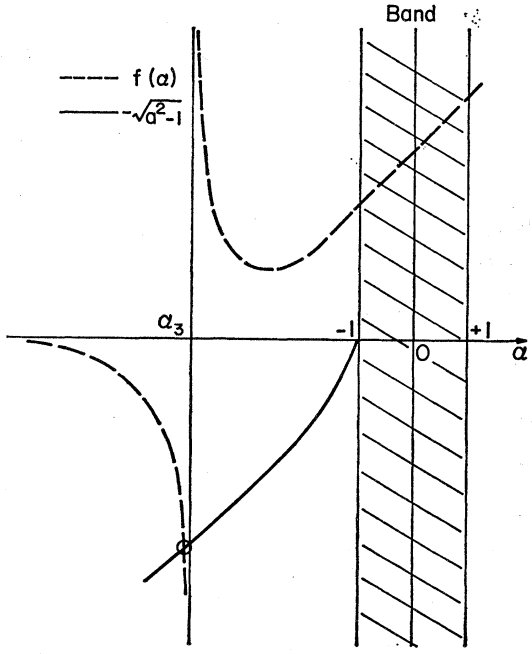

FIG. 3. This is a picture of Eq. (5.7) corresponding to the conditions in Fig. 2, namely, where $f(\alpha)$ never crosses the α axis. The circle shows a bound state.

[5] C. Herring, in *Magnetism*, edited by H. Suhl and G. Rado (Academic Press Inc., New York, 1966), Vol. IV, p. 170. In the same vein, the loop model may also be regarded as a particular two-dimensional system, and for this reason escapes the Lieb-Mattis theorem.

[6] In what follows, the various types of terms that appear in second quantization of the two-body potential have arbitrary coefficients, e.g., U in Eq. (1.2), J in Eq. (1.3), and J', D, and S in Eq. (6.1). The stability of the ferromagnetic eigenstate is then obtained by having these coefficients obey certain inequalities. It may be thought that by so doing one is inadvertently introducing spin-dependent potentials, and that the Lieb-Mattis theorem would not apply for this reason. An argument against this interpretation of the potential coefficients could be made as follows. The various parameters U, J, J', D, S, have one relation among them if the Wannier functions used in their definition are real, namely $D=J$. Thus U, J, J', and S are independent in the sense that the integrals defining them cannot be derived one from any of the others. Therefore, we can always imagine that a potential V is a sum of obviously spin-independent functions V_i: $V=c_1V_1+c_2V_2+c_3V_3+c_4V_4$, and then determine the four constants c_i $(i=1,2,3,4)$ by forcing the integrals U, J, J', and S to have their prescribed values. Figures 12 and 15 exhibit the results of numerical calculations which exhibit a stable ferromagnetic eigenstate when $D=J$.

[7] See, for example, M. Bailyn, Phys. Rev. **139**, A1905 (1965).

[8] J. Hubbard, Proc. Roy. Soc. (London) **A276**, 238 (1963), and subsequent articles.

[9] E. Lieb and F. Wu, Phys. Rev. Letters **20**, 1445 (1968).

[10] J. C. Slater, G. Koster, and H. Statz, Phys. Rev. **91**, 1323 (1953).

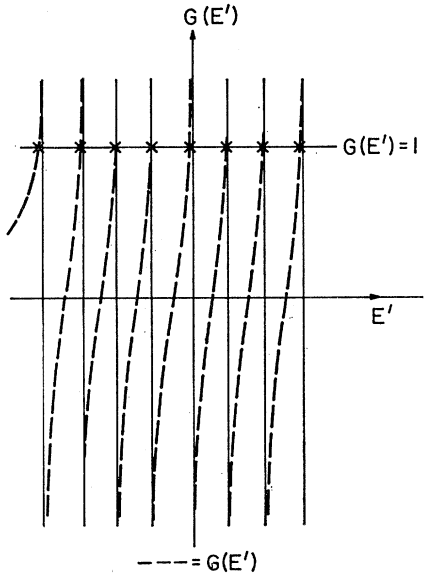

FIG. 4. The continuum part of Eq. (5.4) under the conditions of paragraph (2) below Eq. (5.8).

ing Heisenberg term emerges:

$$H_{\rm ex}=\sum_{ij}{}' [J_{ij}{}^{(xy)}(c_{i+}{}^{\dagger}c_{i-}c_{j-}{}^{\dagger}c_{j+}+c_{i-}{}^{\dagger}c_{i+}c_{j+}{}^{\dagger}c_{j-}) +\tfrac{1}{2}J_{ij}{}^{(z)}(n_{i+}-n_{i-})(n_{j+}-n_{j-})]. \quad (1.3)$$

We have separated the $J^{(xy)}$ from the $J^{(z)}$ part for convenience in tracing the effects. There are three other kinds of two-site interactions.[11] These terms are discussed in Sec. 6. They do not alter the essential results obtained from Eqs. (1.1)–(1.3).

The Hamiltonian

$$H=H_b+H_c+H_{\rm ex} \quad (1.4)$$

has been used by a number of authors as a model for understanding the magnetic properties of metallic systems. See for example Ref. 12 and references listed there. The calculations usually made have the advantage of dealing with arbitrary spin and contain the thermodynamics directly but have the disadvantage of obtaining solutions via the random phase approximation or some variation thereof.

The approach used here expands the wave function in a complete set of elementary single electron-hole excitation states (which therefore specifies the spin) and solves for the coefficients. This can be done without approximation.[13] We do not calculate the thermodynamic functions in this paper.

[11] M. Bailyn, Advan. Phys. **15**, 179 (1966), Sec. 1.3.3.

[12] J. F. Cornwell, Proc. Roy. Soc. (London) **284**, 423 (1965). See also Ref. 1.

[13] The authors are indebted to Professor A. J. Freeman for commenting on their solution and reminding them of the early work of Slater, Koster, and co-workers. In fact, the method of approach used in this paper is identical to that found in Ref. 10, and had the authors of that article considered the electron-hole excitation and included $H_{\rm ex}$ explicitly in their calculations, they would have come across the results we present here. In fact, it is a little surprising to us that apparently no one before now has considered the electron-hole excitation from this point of view.

In Sec. 2 the general problem is formulated, using Eq. (1.4), and in Sec. 3 the solution is obtained in terms of two branches A and B of the spectrum. Branch A is discussed in detail in Sec. 4 and Branch B in Sec. 5. The additional terms needed to make the complete Coulomb interaction are discussed in Sec. 6. Numerical calculations are described in Sec. 7, and a summary of results and a general discussion presented in Sec. 8.

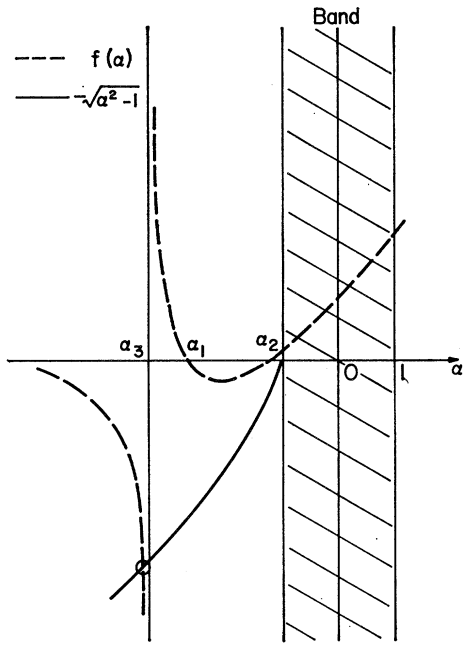

FIG. 5. Equation (5.7), under the same conditions as in Fig. 4, namely, that $f(\alpha)$ crosses the α axis twice, but to the left of the continuum.

2. FORMULATION

In this section we set up the Schrödinger equation for spin $\frac{1}{2}N-1$ and reduce it to a set of difference equations. The one-dimensional model Hamiltonian including nearest-neighbor spin, band, and direct Coulomb repulsion terms, for N sites on a circle is obtained from Eq. (1.4). In H_b, the same-site V_{ii} energy is set equal to zero, and all energies are henceforth measured relative to it. The nearest-neighbor V_{ij} is called V, and becomes a basic parameter in the theory. Thus we deal with

$$H=V\sum[c_{i\sigma}{}^{\dagger}c_{i+1,\sigma}+c_{i+1,\sigma}{}^{\dagger}c_{i\sigma}]+U\sum n_{i+}n_{i-}+J^{(x-y)} \times\sum[c_{i+}{}^{\dagger}c_{i-}c_{i+1,-}{}^{\dagger}c_{i+1,+}+c_{i-}{}^{\dagger}c_{i+}c_{i+1,+}{}^{\dagger}c_{i+1,-}] +\tfrac{1}{2}J^{(z)}\sum(n_{i+}-n_{i-})(n_{i+1,+}-n_{i+1,-}). \quad (2.1)$$

As the ground state $|0\rangle$ we choose the case where all the N electrons have down spin so that $J^{(z)}<0$. The

energy in this state is

$$E_0=\langle 0|H|0\rangle=\tfrac{1}{2}NJ^{(z)}. \tag{2.2}$$

Since the Hamiltonian commutes with the total spin of the system, the simplest stable excitation will be where $N-1$ electrons have down spins, and one electron has an up spin. We try to solve the Schrödinger equation (H−E) $\Psi=0$ by a function of the form

$$\Psi=\sum_{f,g} A_{f,g}\Psi_{f,g}, \tag{2.3}$$

where

$$\Psi_{f,g}=c_{f+}{}^{\dagger}c_{g-}|0\rangle, \tag{2.4}$$

and where the $A_{f,g}$'s are constants to be determined, but which satisfy the periodic boundary conditions

$$\begin{aligned} A_{f+N,g}&=A_{f,g},\\ A_{f,g+N}&=A_{f,g}. \end{aligned} \tag{2.5}$$

Substituting Eq. (2.3) into the Schrödinger equation and taking the matrix element of the result with

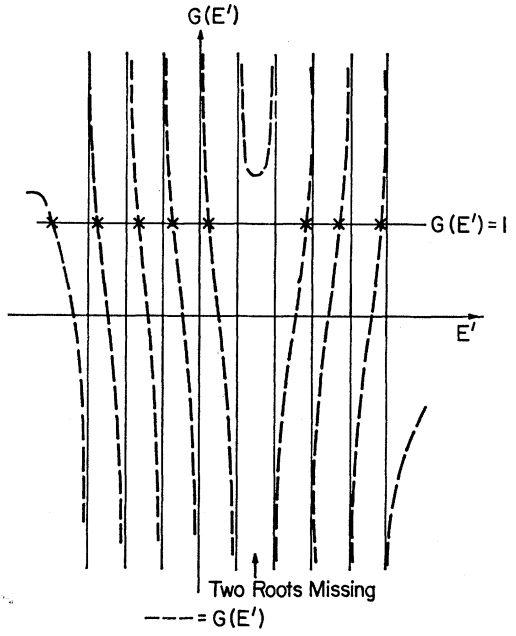

FIG. 6. The continuum part of Eq. (5.4) under the conditions of paragraph (3) below Eq. (5.8). Notice the continuum state lost *inside* the band. *Correction made in proof.* The arrow should read "One Root Missing."

respect to $\Psi_{f,g}$, we get a set of equations:

$$\begin{aligned} V[&A_{f-1,g}+A_{f+1,g}-A_{f,g-1}-A_{f,g+1}]\\ &+J^{(xy)}\delta_{f,g}(A_{f+1,g+1}+A_{f-1,g-1})\\ &+\tfrac{1}{2}J^{(z)}(\delta_{f,g+1}+\delta_{f+1,g})A_{f,g}\\ &-U\delta_{f,g}A_{f,g}-E'A_{f,g}=0, \end{aligned} \tag{2.6}$$

where

$$E'=E-E_0-U+2J^{(z)}. \tag{2.7}$$

In Eq. (2.7) both indices f and g run from 1 through N. There are altogether N^2 such equations. To solve these equations, we try solutions of the form

$$A_{f,g}=\exp(iK(f+g))B_{f-g}(K), \tag{2.8}$$

where

$$K=\pi n/N, \quad n=1, 2, \ldots, N \tag{2.9}$$

and where the Fourier transform of B_r is

$$B_r(K)=N^{-1}\sum_k b_k(K)\exp[ik(f-g)], \tag{2.10}$$

$$r=-\tfrac{1}{2}N+1, \ldots, \tfrac{1}{2}N, \tag{2.11}$$

where N is assumed even.

In order for the $A_{f,g}$ in Eq. (2.8) to satisfy the boundary conditions of Eq. (2.5), we need for each K [i.e., for each n, from Eq. (2.9)]

$$B_{r+N}(K)=(-1)^n B_r(K). \tag{2.12}$$

To accommodate this condition, we require that the k values used in Eq. (2.10) must depend on whether n is odd or even in the following way:

$$\begin{aligned} k&=N^{-1}2\pi m && m=1, 2, \ldots, N, \quad n \text{ even}\\ &=N^{-1}2\pi(m+\tfrac{1}{2}), && m=1, 2, \ldots, N, \quad n \text{ odd}. \end{aligned} \tag{2.13}$$

With this choice of K and k values, we have a well-defined transformation to center of position, $\frac{1}{2}(f+g)$, and relative position, $f-g$, coordinates preserving the periodic boundary conditions. (For an analogous discussion, see Ref. 4, p. 140.) Hereafter, we shall not specify whether n is odd or even, but it will be under-

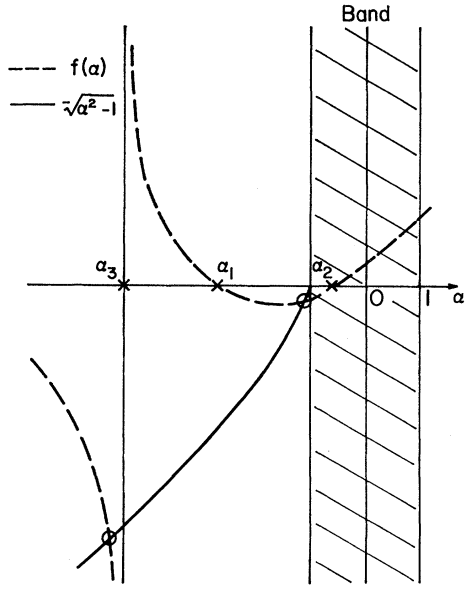

FIG. 7. Equation (5.7), under the same conditions as in Fig. 6, namely, that $f(\alpha)$ crosses the α axis twice, once below and once inside the continuum. The second zero occurs right where the continuum state is missing in Fig. 6. The lost state there is compensated by an additional bound state in this figure.

stood that the selection in Eq. (2.13) is always implied. We write from now on B_r and b_k instead of $B_r(K)$ and $b_k(K)$, respectively.

Putting Eq. (2.8) into Eq. (2.6), and simplifying, we get

$$2iV\sin K(B_{r+1}-B_{r-1})+\delta_{r,0}(2J^{(xy)}\cos 2K-U)B_r +\tfrac{1}{2}J^{(z)}(\delta_{r,1}+\delta_{r,-1})B_r=E'B_r. \quad (2.14)$$

For each of the NK's, Eq. (2.14) is a set of N difference equations, $r=-\frac{1}{2}N+1, \ldots, \frac{1}{2}N$. The problem is now to solve these equations.

3. GENERAL SOLUTION

In this section we obtain the general solution of Eq. (2.14). Let us first define a Fourier transform of B_r

$$b_k=\sum_{r=1}^{N} B_r\exp(ikr), \qquad B_r=N^{-1}\sum_k \exp(-ikr)b_k. \quad (3.1)$$

Multiplying Eq. (2.14) by e^{ikr} and summing over r, we find

$$b_k=[\tfrac{1}{2}J^{(z)}(e^{ik}B_1+e^{-ik}B_{-1})+\eta B_0](E'-E_k)^{-1} \quad (3.2)$$

and from Eq. (3.1).

$$B_r=N^{-1}\sum_k [\tfrac{1}{2}J^{(z)}(e^{-ik(r-1)}B_1+e^{-ik(r+1)}B_{-1}) +\eta e^{-ikr}B_0](E'-E_k)^{-1}, \quad (3.3)$$

where

$$\eta=2J^{(xy)}\cos 2K-U, \qquad E_k=4V\sin K\sin k. \quad (3.4)$$

The E_k are in fact the unperturbed ($U=J^{(z)}=J^{(xy)}=0$) excitation energies.

For $r=1, 0, -1$, Eq. (3.3) yields three homogeneous equations in the three unknowns B_{-1}, B_0, B_1:

$$\begin{aligned} B_1&=\tfrac{1}{2}J^{(z)}uB_1-\eta vB_0+\tfrac{1}{2}J^{(z)}wB_{-1},\\ B_0&=\tfrac{1}{2}J^{(z)}vB_1+\eta uB_0-\tfrac{1}{2}J^{(z)}vB_{-1},\\ B_{-1}&=\tfrac{1}{2}J^{(z)}wB_1+\eta vB_0+\tfrac{1}{2}J^{(z)}uB_{-1}, \end{aligned} \quad (3.5)$$

where

$$u=u^*=\frac{1}{N}\sum_k (E'-E_k)^{-1},$$

$$v=-v^*=\frac{1}{N}\sum_k (E'-E_k)^{-1}e^{ik}, \quad (3.6)$$

$$w=w^*=\frac{1}{N}\sum_k (E'-E_k)^{-1}e^{2ik}.$$

The determinantal equation for nontrivial roots of Eq. (3.5) can be set up, multiplied out, and without difficulty reduced to the product

$$\tilde{F}\tilde{G}=0, \quad (3.7)$$

where

$$\tilde{F}\equiv\tfrac{1}{2}J^{(z)}(u+w)-1=0 \quad (3.8)$$

represents branch A of solutions, and

$$\tilde{G}\equiv\tfrac{1}{2}J^{(z)}\{\eta(u^2-uw+2v^2)+w-u\}-\eta u+1=0 \quad (3.9)$$

represents branch B of solutions.

It can be shown that $\tilde{F}=0$ when substituted into Eq. (3.5) leads to

$$B_0{}^{(A)}=0 \quad B_1{}^{(A)}-B_{-1}{}^{(A)}=0, \quad (3.10)$$

whereas $\tilde{G}=0$ leads to

$$B_0{}^{(B)}\neq 0 \quad B_1{}^{(B)}=-B_{-1}{}^{(B)}\cdots. \quad (3.11)$$

This symmetry is rather peculiar: The relative wave functions B_r are either antisymmetric or symmetric upon $r\leftrightarrow -r$ provided $r\neq 0$, but if $r=0$, the *symmetric* one vanishes. There will be one exception to Eq. (3.11): the "exciton" state for $K=0$ in branch B will have $B_0=0$. (See Ref. 14.)

Some insight into why this type of symmetry occurs can be gained by going back to Eq. (2.14) and setting $J^{(xy)}=J^{(z)}=U=0$. The equation then reduces to a very simple one, and it is easily seen that the Bloch function for the relative distance r, $\exp(-ikr)$, is a solution with energy E_k. Now the usual symmetry and antisymmetry would occur if $E_{-k}=E_k$, but this is not

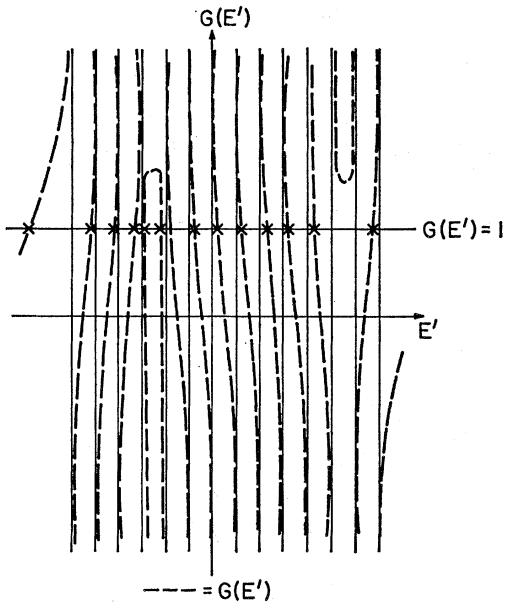

FIG. 8. The continuum part of Eq. (5.4) under the conditions of paragraph (4) below Eq. (5.8). Notice the continuum state lost and the continuum state gained.

[14] The bound exciton state for $K=0$ (in branch B) is the one exception. In this case, only B_1 and B_{-1} are not zero, so Eq. (5.13) cannot be used. Whenever $B_0\neq 0$, (i.e., in all other cases), Eq. (5.13) can be used.

the case[15] [see Eq. (3.4)]. Rather, $E_{-k}=-E_k$. But with K as a fixed parameter the same energy is obtained for k and $\pi-k$. It can be shown that two combinations of $\exp(ikr)$ and $\exp(i(\pi-k)r)$ that satisfy the boundary conditions are

$$B_r^{(A)}=i^r\sin(k-\tfrac{1}{2}\pi)r,$$
$$B_r^{(B)}=i^r\cos(k-\tfrac{1}{2}\pi)r. \tag{3.12}$$

These functions *do* have the peculiar symmetry indicated in Eq. (3.10) and (3.11). Notice that if the factors i^r were not there we would have the usual symmetry, but by the same token, we would not have $B_r\equiv\pm B_{r+N}$.

4. SOLUTION OF BRANCH *A*

Here we describe in detail the nature of the solutions of branch A obtained by setting $\tilde{F}=0$. By definitions of u and w, Eq. (3.6), the equation (3.8) becomes after some slight manipulation and definition of F:

$$F(E')\equiv\tfrac{1}{2}J^{(z)}(u+w)$$
$$=N^{-1}\sum_k\frac{J^{(z)}\cos^2k}{E'-E_k}=1. \tag{4.1}$$

Let us examine $F(E')$. If $J^{(z)}<0$, then for each particular E_k, except the one where $\cos k=0$, i.e., $k=\frac{1}{2}\pi$, $F(E')$ suffers an infinite discontinuity as shown schematically in Fig. 1. The dotted lines represent the function $F(E')$, the vertical lines represent discrete values of E_k's. The intersections of dotted line with $F=1$ are the solutions of Eq. (4.1) and give the energy eigenvalues. There are altogether $\frac{1}{2}N-1$ such roots; $\frac{1}{2}N-2$ lie in the "continuum" (or band), and another one lies outside the continuum. The latter is of special interest.[16]

To see the features of the state below (or above) the band, we convert the sum in Eq. (4.1) to an integral (justified by the fact that the solution of E' lies out of the range of E_k)

$$N^{-1}\sum_k=(2\pi)^{-1}\int_{-\pi}^{\pi}dk \tag{4.2}$$

and introduce the abbreviations

$$\alpha\equiv E'/\xi, \tag{4.3}$$

$$\xi\equiv(4V\sin K). \tag{4.4}$$

The continuum region is then given by $-1<\alpha<1$, and

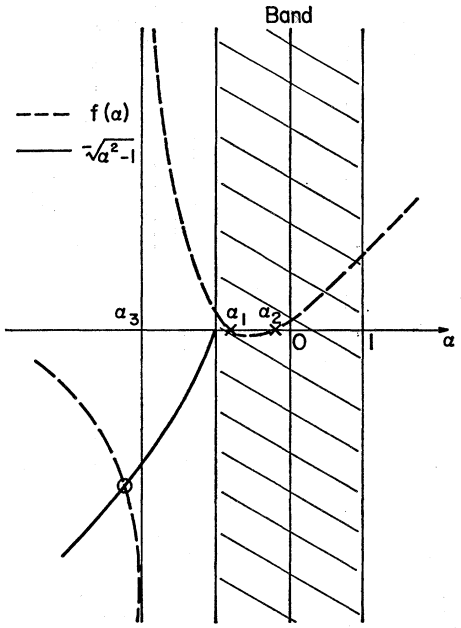

FIG. 9. Equation (5.7) under the same conditions as in Fig. 8, namely, that $f(\alpha)$ crosses the α axis twice, both times inside the continuum. The lost and gained continuum states in Fig. 8 occur where the zeros of $f(\alpha)$ appear in this figure.

Eq. (4.1) becomes

$$F(E')=J^{(z)}\xi^{-1}\frac{1}{2\pi}\int_{-\pi}^{\pi}dk\frac{\cos^2k}{\alpha-\sin k}$$
$$=J^{(z)}\xi^{-1}[\alpha+(\alpha^2-1)^{1/2}]=1,\quad \alpha<-1 \tag{4.5}$$

where for now we have assumed $\xi>0$ and looked for roots $\alpha<-1$.

In Eq. (4.5), the factor $\alpha+\sqrt{\alpha^2-1}$ is always less than 1 in magnitude for $\alpha<-1$. Thus there can be a solution to Eq. (4.5) only if $|J^{(z)}/\xi|$ satisfies

$$|J^{(z)}/\xi|>1. \tag{4.6}$$

If this is satisfied then the solution is

$$\alpha=\tfrac{1}{2}J^{(z)}\xi^{-1}[1+(J^{(z)}/\xi)^{-2}]. \tag{4.7}$$

The energy is obtained using Eqs. (4.3) and (2.7), and is written below in Eq. (8.2). Equations (4.6) and (4.7) are also true for $\xi<0$.

Next let us consider the correlation function $|B_r|^2$ which is proportional to the probability that the electron-hole pair is separated by a distance r. From Eqs. (3.3) and (3.10), integrating over k as before for the solution below the band, we find

$$B_0^{(A)}=0,$$
$$B_r^{(A)}=(-i)^{r-1}\left(\frac{1}{|J^{(z)}/\xi|}\right)^{r-1}B_1,\quad r\geq1. \tag{4.8}$$

Thus when Eq. (4.6) is satisfied, the function $|B_r|^2$ decreases exponentially with increasing r, and the

[15] This does not violate time reversal symmetry, because there are two wave vectors involved, k and K. If the energy in Eq. (3.3) is called $E_{k,K}$ then $E_{-k,K}=E_{k,K}$. What is under discussion here is that $E_{-k,K}=-E_{k,K}$.

[16] The splitting off of states from the continuum is analogous to the splitting off of bound states in the impurity problem. See, for example, G. Koster and J. C. Slater, Phys. Rev. **95**, 1167 (1954); **96**, 1208 (1954).

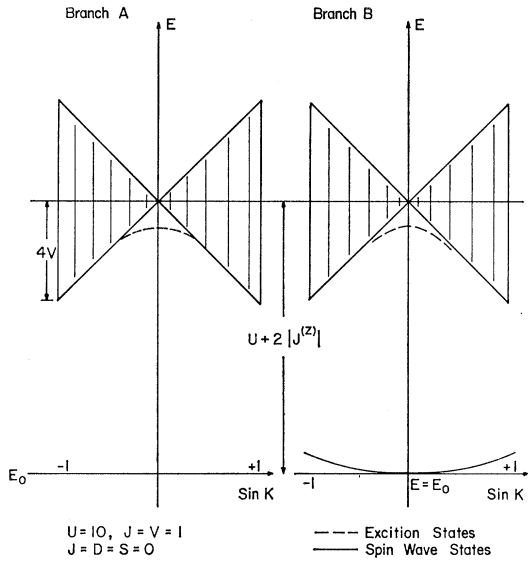

FIG. 10. This is a schematic plot of a typical energy versus sin$K$ spectrum; the shaded region indicates the spread of continuum states, the dashed lines indicate the exciton states, and the solid curve represents the spin-wave spectrum. This summarizes the results of Secs. 4 and 5. *Correction made in proof.* The J on the bottom line should be a J'.

state below the continuum has the true physical significance of a bound state (electron bound to hole). As $|J^{(z)}/\xi| \to 1$, Eq. (4.8) shows that the wave function becomes spread out over the whole crystal, which is just the characteristic of a continuum state. If $|J^{(z)}/\xi|$ becomes $=1$, then the conversion from a sum to an integral as in Eq. (4.2) is no longer valid. The bound state has then reverted to an ordinary band state but occupying the lowest energy of the band.

Where a bound state does exist, it has zero probability of having the excited electron over the hole. This state does not correspond to the originary spin wave, and is not a generalization of one. It is a kind of exciton excitation below the continuum, and we shall call it by this name.

5. SOLUTION OF BRANCH *B*

In this section we investigate the solutions of branch B. From Eq. (3.9) the dispersion relation for branch B is

$$G(E')\equiv 1-\tilde{G}=\eta u+J^{(z)}\tfrac{1}{2}(u-w) -\tfrac{1}{2}J^{(z)}\eta(u^2-uw+2v^2)=1. \quad (5.1)$$

By definitions of u, v, w, Eq. (3.6), $G(E')$ can be rewritten as

$$G(E')=\frac{1}{N}\sum_k \frac{J^{(z)}\sin^2 k+\eta}{E'-E_k} - \frac{1}{N^2}\sum_{k,q}\frac{\tfrac{1}{2}J^{(z)}\eta(\sin k-\sin q)^2}{(E'-E_k)(E'-Eq)}=1.$$

After some manipulation, this reduces to

$$G(E')=\frac{1}{N}\sum_k \frac{2x\sin^2 k-2xy\sin k+y}{\alpha-\sin k}=1, \quad (5.2)$$

where

$$x\equiv \tfrac{1}{2}J^{(z)}/\xi, \quad y\equiv \eta/\xi, \quad \eta=2J^{(xy)}\cos 2K-U, \quad (5.3)$$

and where α and ξ are defined in Eqs. (4.3) and (4.4).

Let us now investigate the general feature of $G(E')$ as we have done for branch A, and restrict ourself to the cases $J^{(z)}<0$, and $\eta<0$. ($\eta<0$ is true as long as U is large; and $J^{(z)}<0$ is the ferromagnetic case for which the ground state is designed.) The other cases can be treated in a similar fashion without much alteration. Thus we will have either $x<0$, $y<0$, or $x>0$, $y>0$.

Equation (5.2) can be rewritten, after further manipulation, as follows:

$$G(E')-1=g(\alpha)N^{-1}\sum_k(\alpha-\sin k)^{-1} -2x(\alpha-\alpha_3)=0, \quad (5.4)$$

where

$$g(\alpha)=2x\alpha^2-2xy\alpha+y=2x(\alpha-\alpha_1)(\alpha-\alpha_2), \quad (5.5)$$

where

$$\alpha_1=\tfrac{1}{2}y[1+(1-2/xy)^{1/2}], \quad \alpha_2=\tfrac{1}{2}y[1-(1-2/xy)^{1/2}], \quad \alpha_3=y(1-1/2xy)\ . \quad (5.6)$$

We next look for states whose energies lie below the band. When $\xi>0$, then $\alpha<-1$, and when $\xi<0$, then $\alpha>1$ correspond to the regions where these low-lying states must lie. We get from Eq. (5.4) for these two cases, converting the sum to an integral over k,

$$f(\alpha)\equiv(\alpha-\alpha_1)(\alpha-\alpha_2)(\alpha-\alpha_3)^{-1} =-(\alpha^2-1)^{1/2}\cdots\alpha<-1, \quad (5.7)$$

$$f(\alpha)\equiv(\alpha-\alpha_1)(\alpha-\alpha_2)(\alpha-\alpha_3)^{-1} =+(\alpha^2-1)^{1/2}\cdots\alpha>1. \quad (5.8)$$

It can be easily proved for $x<0, y<0$, that $\alpha_3\leq\alpha_1\leq\alpha_2$, and for $x>0, y>0$, that $\alpha_3\geq\alpha_1\geq\alpha_2$. Further, for a given pair of x and y, Eqs. (5.7) and (5.8) cannot have real solutions in the allowed α ranges simultaneously.

Let us now look at the qualitative aspects of the solutions in terms of the roots, α_1, α_2, of $g(\alpha)$. Further let us choose $\xi>0$ (the other case $\xi<0$ gives identical results). This means $x<0$, $y<0$. The following possibilities occur.

(*1*) $g(\alpha)=0$ *has no real roots.* Since $x<0$, $g(\alpha)<0$ for all values of α. A qualitative graph of $G(E')$ versus E' in and near the continuum, from Eq. (5.4) is shown in Fig. 2, and a corresponding graph of $f(\alpha)$, Eq. (5.7), is shown in Fig. 3. In this case there is only one solution to $G=1$ below the band, shown in the circle in Fig. 3.

(*2*) $g(\alpha)$ *has real roots, but both lie below the band.* The function $g(\alpha)$ is less than zero over the entire interval $(-1, 1)$, and there is only one solution to $G=1$ below the band. The situation is also illustrated by Figs. 4 and 5.

(3) $g(\alpha)$ *has only one root,* α_2*, lying in the band.* It follows that $g(-1)>0$. The function $g(\alpha)$ changes sign at α_2; let $\alpha_2=\sin k_0+e$, $e=\lambda(2\pi/N)\cos k_0$ and $0<\lambda<1$, for some particular k_0 in the band. A qualitative graph of $G(E')$ is shown in Fig. 6. The minimum of the turn-up portion of $G(E')$ can be shown to be greater than 1. The proof is given in Appendix A, hence one solution to $G(E')=1$ inside the band is missing and there is an extra solution to $G=1$ outside the band. This means that two roots of $G=1$ lie below the band. Figure 7 illustrates the graph of Eq. (5.7), and the circles show the two roots below the band.

(4) *Both roots of* $g(\alpha)$, α_1 *and* α_2*, lie inside the band.* A graph of $G(E')$ is shown in Fig. 8. There is a turn-up portion of the $G(E')$ curve, and also a turn-down portion. It can also be shown that both the minimum of the turn-up portion and the maximum of the turn-down portion of $G(E')$ are greater than 1, and hence one state inside the band has shifted its position. There is only one solution to Eq. (5.7). Figure 9 illustrates this situation.

From the graphs, we can see that there is always one solution lying below α_3, and whenever there are more than one solution, the extra root to Eq. (5.4) produced by the entry of α_2 into the band lies close to the band edge. The lower root is a generalized spin wave, and the other one, when it occurs, is an exciton similar in many respects to the bound state of branch A.

The root of Eq. (5.7) which lies below α_3 will be called α_s. The index symbolizes that it is a generalized spin wave. Since $|\alpha_3|$ is in general a large number, and $|\alpha|>|\alpha_3|$, we can use the following approximation[17] to simplify Eq. (5.7):

$$(\alpha_s^2-1)^{1/2}\cong-\alpha_s\left(1-\frac{1}{2\alpha_s^2}\right),\quad \alpha<-1. \tag{5.9a}$$

[If we do not use Eq. (5.9a) we could solve Eq. (5.7) exactly, but the general solution is extremely complicated.] Equation (5.7) becomes, with use of Eq. (9.4), a quadratic rather than a cubic equation:

$$\alpha_s^2-(x+y)\alpha_s+(xy-\tfrac{1}{2})=0.$$

One root of this equation does not satisfy $\alpha<\alpha_3$. The other is[18]

$$\alpha_s=\tfrac{1}{2}\{x+y-[(x-y)^2+2]^{1/2}\}\cong y-[2(x-y)]^{-1}. \tag{5.9b}$$

From Eqs. (2.6) and (5.3) we get

$$E_s=E_0+(-2J^{(z)}+2J^{(xy)}\cos 2K)-8V^2\sin^2K[U-(2J^{(xy)}\cos 2K-\tfrac{1}{2}J^{(z)})]^{-1}. \tag{5.10}$$

[17] Using Eqs. (4.3), (4.4), and (2.7), we get $\alpha=(E-E_0-U-2J)/4V\sin K$, where we set $J^{(xy)}=J^{(z)}=-J$. It can be proved rigorously from Eq. (5.7) that as $K\to 0$, the lowest root $E_s\to E_0$. Thus $\alpha_s\to\infty$, and the approximation in Eq. (5.9) is justified. As $\sin K\to 1$, however, we must content ourselves with considering α_3, which in this limit approaches $-\frac{1}{4}U/V-4V/J+\frac{1}{2}J/V$. One way to get this large in magnitude is to set $U\gg V$, and $U>2J$. Under these conditions, Eq. (5.9) is approximately valid for all K.

[18] Here the approximation is $|y-x|\gg 2$. Once again this can be shown to be rigorously valid in the limit $K\to 0$, and approximately valid for all K provided $U\gg V$ and $U>2J$. Thus Eqs. (5.10) and (5.11) will be valid under these conditions.

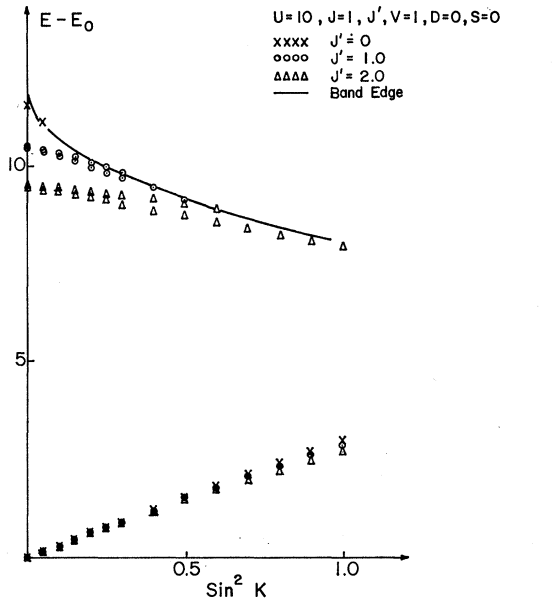

FIG. 11. In this figure, the lower edge of the band, the excitons, and the spin-wave spectrum are plotted versus $\sin^2K$ for fixed U, J, V, D, and S and variable J'. See Eq. (6.14) and Sec. 7. The band edges are indistinguishable for the different J''s and the spin waves are almost so.

The first term is the F-eigenstate energy.[19] The second term is the ordinary spin-wave energy $\sim 1-\cos 2K$. The third term is essentially *negative* and represents the loss in kinetic energy allowed by having one electron with up-spin (for in the F eigenstate this electron had to sit on top of the down-spin Fermi distribution). This last term is the greater in magnitude the greater the Bloch bandwidth ($\sim V$) is. If V gets sufficiently large, E_s will become lower in algebraic value than E_0, i.e., the system prefers to be in the excited state, and the ferromagnetic eigenstate is unstable. The criterion for this to happen is, setting $J^{(xy)}=J^{(z)}=-J$, and setting the denominator in Eq. (5.10) equal to its smallest value $U-\frac{5}{2}J$,

$$V>[\tfrac{1}{2}J(U-\tfrac{5}{2}J)]^{1/2},\quad \text{ferromagnetic eigenstate unstable, } U \text{ large}. \tag{5.11}$$

This is then a criterion[18] for the instability of the ferromagnetic eigenstate. Further, if $J=0$, the ferromagnetic state can never be the ground state no matter how large U is: This can be seen directly by substituting $x=0$ in Eq. (5.2). The result is $\alpha=-[(1+y)^{1/2}]^2$, i.e., $E=U[1-(1+y^{-2})^{1/2}]\leq 0$, and the ferromagnetic eigenstate energy is zero.

Now let us calculate the correlation function for the bound states of branch B. Inserting $B_1=-B_{-1}$, $B_0\neq 0$

[19] The term "F eigenstate" used hereafter actually denotes the saturated ferromagnetic eigenstate, $|0\rangle$.

into Eq. (3.5) we get

$$B_1=\frac{\eta v}{\frac{1}{2}J^{(z)}(u-w)-1}B_0. \tag{5.12}$$

Substituting Eq. (5.12) into Eq. (3.3), and changing the summations over k into the corresponding integrals, we have the following result[14]:

$$|B_r|^2=|B_0|^2[\alpha+(\alpha^2-1)^{1/2}]^{2r},\quad \alpha<-1,\quad r\geq 0. \tag{5.13}$$

This represents electron-hole bound states with wave functions having a peak at $r=0$, and falling off exponentially with increasing r. (Contrast this with the exciton of branch A which had $B_0=0$, but otherwise fell off exponentially.) For the exciton here, the only restriction is that $\alpha<-1$, i.e., that it lies below the continuum. This criterion ends up being very similar to the one for the exciton of branch A, and is written out in Eq. (8.4) below. There may be a cutoff here also.

The spin-wave state by definition has the lowest root of Eq. (5.7), and always lies below the exciton; and in fact at $K=0$, the spin-wave energy must be zero. So at least a part of the spin-wave spectrum will always appear. The higher K part of the spectrum may, however, merge with the continuum if $\alpha_s=-1$, where α_s is obtained exactly by solving Eq. (5.7), or approximately[18] from Eq. (5.10). In the latter case the merging occurs when

$$\sin K=\frac{U}{4(V+J\cos K)}+\frac{4V''^2}{-J}\frac{\sin^2 2K}{V+J\cos K}, \tag{5.14}$$

provided the right-hand side is less than 1. Otherwise the merging will not occur, in this approximation.

Finally, it can easily be shown that when one operates on the wave functions for these excitations with S^2, the result is

$$S^2\psi=(\tfrac{1}{2}N-1)(\tfrac{1}{2}N)\psi$$

for all states except the one $K=0$ in the spin-wave branch. For this case

$$S^2\psi=\tfrac{1}{2}N(\tfrac{1}{2}N+1)\psi,\qquad K=0 \text{ spin wave}.$$

This follows because of the form of the wave function, which in fact for this state has only one component B_0. Thus for certain values of U, J, etc., the state of lowest energy is the $K=0$ state of the spin-wave branch and has $S=\frac{1}{2}N$ which equals $M+1$, since $M=\frac{1}{2}N-1$. Thus in the subspace $M=\frac{1}{2}N-1$ the lowest-energy state has $S=M+1$. In the proof of the Lieb-Mattis theorem,[4] as mentioned in the Introduction it is necessary to establish that the state of lowest energy of a subspace of given M has $S=M$. Thus we have here an apparent disagreement with the LM theorem. For a fuller discussion, see the Introduction.

6. COMPLETE COULOMB INTERACTION

The object of this section is to analyze the effect of those two-body electrostatic terms that are not included in the Hamiltonian of Eq. (1.7). A general classification of the two-body terms can be found in Ref. 8. Those terms that are not included in the Hamiltonian of Eq. (1.7) are the following:

$$\begin{aligned}H_1&=H_{J'}+H_D+H_S\\&=J'\sum_{i=1}^{N}(n_{i,+}+n_{i,-})(n_{i+1,+}+n_{i+1,-})\\&\quad+D\sum_{i=1}^{N}(c_{i,+}^{\dagger}c_{i+1,+}c_{i,-}^{\dagger}c_{i+1,-}+c_{i,+}^{\dagger}c_{i-1,+}c_{i,-}^{\dagger}c_{i-1,-})\\&\quad+S\sum_{i=1}^{N}\{c_{i,+}^{\dagger}c_{i+1,+}(n_{i,-}+n_{i+1,-})+c_{i,+}^{\dagger}c_{i-1,+}\\&\quad\times(n_{i,-}+n_{i-1,-})+c_{i,-}^{\dagger}c_{i+1,-}(n_{i,+}+n_{i+1,+})\\&\qquad+c_{i,-}^{\dagger}c_{i-1,-}(n_{i,+}+n_{i-1,+})\}.\end{aligned} \tag{6.1}$$

The index D stands for double-hopping, S stands for semihopping, and J' indicates that this term will have an exchange effect. We treat J', D, and S as new parameters in the problem. The new ground-state energy is

$$E_0'=\tfrac{1}{2}NJ^{(z)}+NJ'. \tag{6.2}$$

Proceeding as in Sec. 2, we find now instead of Eq. (2.6) rather

$$\begin{aligned}&V[A_{f-1,g}+A_{f+1,g}-A_{f,g-1}-A_{f,g+1}]-U\delta_{f,g}A_{f,g}+J^{(xy)}\delta_{f,g}(A_{f+1,g+1}+A_{f-1,g-1})+(\tfrac{1}{2}J^{(z)}-J')(\delta_{f,g+1}+\delta_{f,g-1})A_{f,g}\\&\quad-D[\delta_{f,g-1}A_{f+1,g-1}+\delta_{f,g+1}A_{f-1,g+1}]+S(A_{f+1,g}+A_{f-1,g})-S\{(\delta_{f,g}+\delta_{f,g-1})A_{f+1,g}+(\delta_{f,g}+\delta_{f,g+1})A_{f-1,g}\\&\qquad+(\delta_{f,g}+\delta_{f,g-1})A_{f,g-1}+(\delta_{f,g}+\delta_{f,g+1})A_{f,g+1}\}=E'A_{f,g},\end{aligned} \tag{6.3}$$

where $E'\equiv E-E_0'-U+2J^{(z)}$.

Following the same procedure as in Secs. 2 and 3 and defining

$$\mathcal{S}\equiv 2S\cos K, \tag{6.4}$$

$$\xi\equiv 4[(V+S)^2\sin^2 K+S^2\cos^2 K]^{1/2}, \tag{6.5}$$

$$\sin\varphi\equiv\frac{S\cos K}{[(V+S)^2\sin^2 K+S^2\cos^2 K]^{1/2}}=\frac{2\mathcal{S}}{\xi}, \tag{6.6}$$

$$J''=(1/2)J^{(z)}-J', \tag{6.7}$$

we are led to

$$b_k=\frac{(J''e^{ik}-\mathcal{S}-De^{-ik})B_1+(\eta-2\mathcal{S}\cos k)B_0+(J''e^{-ik}-\mathcal{S}-De^{ik})B_{-1}}{E'-\xi\sin(k+\varphi)}, \tag{6.8}$$

which now replaces Eq. (3.2). Defining

$$u\equiv N^{-1}\sum_k\frac{1}{E'-\xi\sin(k+\varphi)}, \tag{6.9}$$

$$X_\varphi\equiv N^{-1}\sum_k\frac{e^{-ik}}{E'-\xi\sin(k+\varphi)}=e^{i\varphi}v, \tag{6.10}$$

$$Y_\varphi\equiv N^{-1}\sum_k\frac{e^{-2ik}}{E'-\xi\sin(k+\varphi)}=e^{2i\varphi}w, \tag{6.11}$$

where u, v, and w are defined in Sec. 3, we are led to three equations [just as we previously were led to Eq. (3.5)] for which the determinantal equation is

$$\Delta\equiv\begin{vmatrix} uJ''-\mathcal{S}X_\varphi-DY_\varphi-1 & \eta X_\varphi-\mathcal{S}(u+Y_\varphi) & J''Y_\varphi-\mathcal{S}X_\varphi-Du \\ J''X_\varphi^*-u\mathcal{S}-DX_\varphi & \eta u-\mathcal{S}(X_\varphi^*+X_\varphi)-1 & J''X_\varphi-\mathcal{S}u-DX_\varphi^* \\ J''Y_\varphi^*-\mathcal{S}X_\varphi^*-Du & \eta X_\varphi^*-\mathcal{S}(u+Y_\varphi^*) & J''u-\mathcal{S}X_\varphi^*-DY_\varphi^*-1 \end{vmatrix}=0. \tag{6.12}$$

In order to investigate the bound states, we replace the k sum by an integral. Then using

$$x\equiv J''/\xi,\quad y\equiv\eta/\xi,\quad z\equiv\mathcal{S}/\xi,\quad d\equiv D/\xi,\quad \alpha\equiv E'/\xi, \tag{6.13}$$

Eq. (6.12) reduces to

$$1/(\alpha^2-1)^{1/2}g(\alpha)+h(\alpha)=0,\quad \alpha<-1 \tag{6.14}$$

where

$$g(\alpha)=8(x^2-d^2)\alpha^3-[8(x^2-d^2)y+16z^2(x-d)+4d]\alpha^2 +[4xy+4z^2-4(x^2-d^2)]\alpha +[4(x^2-d^2)y+8z^2(x-d)+2d-y-2x], \tag{6.15}$$

$$h(\alpha)=8(x^2-d^2)\alpha^2-[8(x^2-d^2)y+16z^2(x-d)+4d]\alpha +[4xy+4z^2-1]. \tag{6.16}$$

Numerical solutions to (the square of) Eq. (6.14) are discussed in Sec. 7.

7. NUMERICAL CALCULATIONS

In this section, numerical results are presented in the form of the Figs. 10–15. Each curve represents a computer solution of Eq. (6.14) with a given set of input parameters $\{U,J,J',V,D,S\}$; here we consider only the ferromagnetic case and let $J^{(z)}=J^{(xy)}=-J\leqq 0$.

The object of this numerical study is to show the effect of various terms on the energy spectrum of the low-lying excited states, particularly the spin-wave states.

In Figs. 11–15 the energy spectrum is plotted as a function of $\sin^2K$, and the lower edge of the band of quasicontinuous states is also shown in each figure. For each value of $\sin^2K$ the separation between the center of the band and the F eigenstate is $U+2J$, and the half-width of the band is ξ ,where

$$\xi=4[(V+S)^2\sin^2K+S^2\cos^2K]^{1/2}.$$

Note that if $\sin^2K=0$ the band has a half-width $\xi_0=4|S|\neq 0$. The figures in general bear a striking resemblance to Slater's in Ref. 1.

Let us first consider the exciton levels. The following is observed:

(i) For $D=0$, the two exciton levels lie very close to each other (Fig. 12).

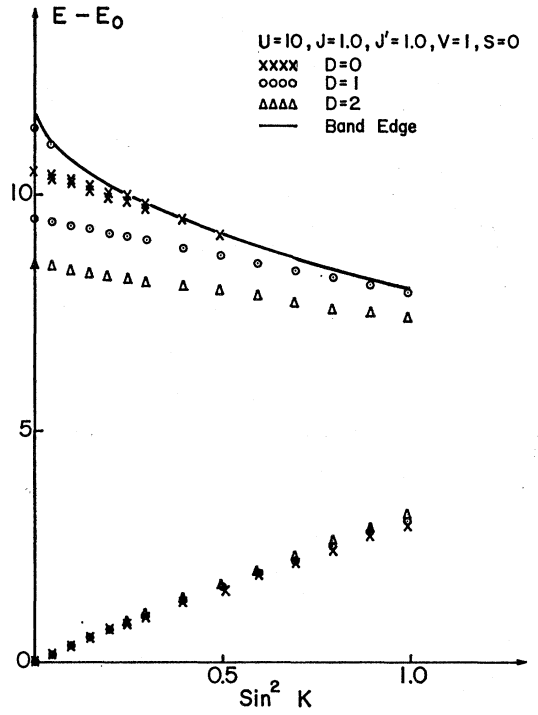

FIG. 12. Similar to Fig. 11, except that J' is fixed and D varies. Again the band edge is indistinguishable for the various D's, and the spin waves almost so.

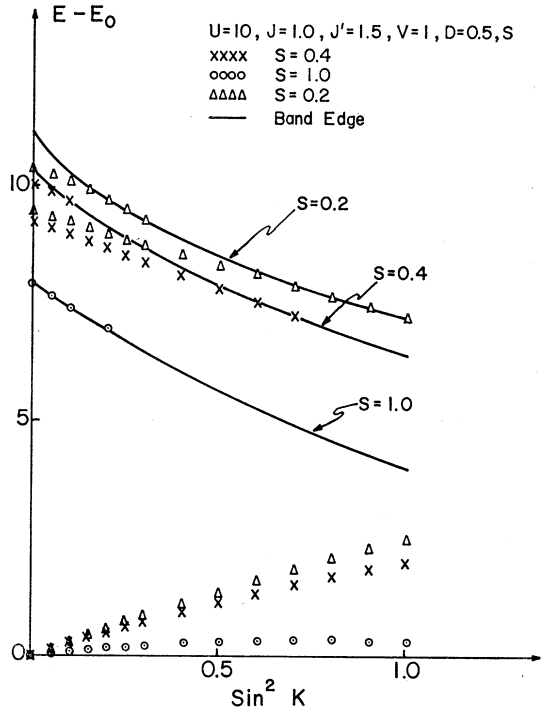

FIG. 13. In this figure, the values of U, J, J', V, and D are fixed with the S value varying. As the value of S varies, the band edge also shifts, so there are three distinct band edges with corresponding S values indicated. Notice the dip the band edge and spin waves take for large S.

(ii) The effect of J' is additive to the effect of $\frac{1}{2}J$ (Fig. 11); this can also be seen analytically from Eq. (6.3).

(iii) The effect of D is to split the two exciton levels (Fig. 12). This can be seen from Eqs. (6.14)–(6.16) for $S=0$ by factoring Eq. (6.14) into two branches again. The one branch contains D in the combination $\frac{1}{2}J^{(z)}+D$ the other in the combination $\frac{1}{2}J^{(z)}-D$.

(iv) The effect of S is to push the exciton levels and lower edge of the band downward, the exciton levels finally merging into the band (Fig. 13).

For the spin-wave spectrum, the following is observed:

(i) $E_s-E_0\rightarrow 0$ as $\sin^2K\rightarrow 0$; this can be proved analytically.

(ii) For relatively large U (Figs. 11–14), and small $\sin^2K$, the spin-wave spectrum is approximately linear in $\sin^2K$, the departure from linearity increases as $\sin^2K$ increases.

(iii) The effect of J' is to turn the spectrum slightly downward (Fig. 11).

(iv) The effect of D is to turn the spectrum slightly upward (Fig. 12).

(v) The effect of S and V are similar; this can be seen by comparing Fig. 14 and Fig. 13. Increasing either one of them or both tends to decrease the slope of this linear portion of the spectrum and enhance the nonlinearity of the spectrum.

(vi) For relatively small U (Fig. 15), all the observations above are still valid; but the effect of S and the nonlinear behavior is more clearly manifested.

(vii) It is possible for the spin-wave energy to become smaller than E_0 at the far end of the spectrum by the downward turn for large K becoming sufficiently large (Fig. 15).

8. SUMMARY

In the previous sections we have set up and solved the Schrödinger equation for the electron-hole excitation on a one-dimensional ferromagnetic ground state including the complete nearest-neighbor Coulomb interaction. The spectrum consists of three types of excitations: band, exciton, and spin wave, for each value of K, the momentum of the center of the electron-hole combination. Let us here review the general features of these solutions, for the case where $S=D=J'=0$. In this case the spectrum splits into two branches A and B as shown in Fig. 10.

First of all, the band states are centered, for every K, at a distance $U+2|J|$ above the ground state E_0 of the ferromagnetic state. The range of energies in the band for each K is $-1<\alpha<1$, or $8V\sin K$, and the energy of the "band" at $K=0$ is exactly $U+2|J^{(z)}|$ from the F-eigenstate energy. (When S is included, the band at $K=0$ spreads out.) The bands may not only have a state dropped off from the bottom (or top) but may have a state removed from the middle, or shifted from one part

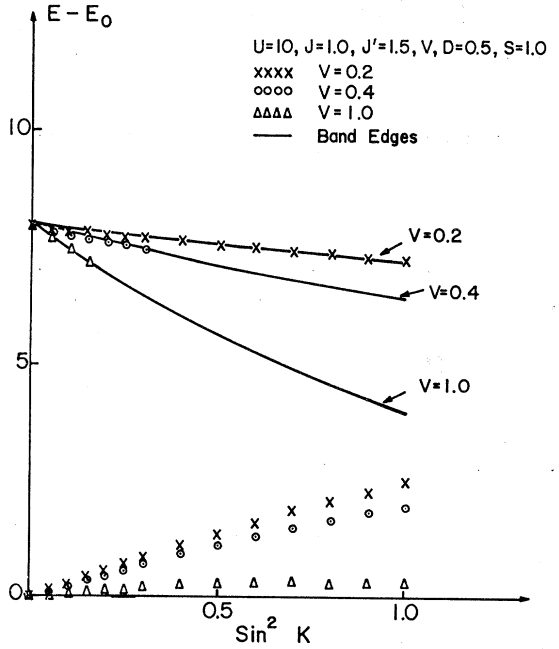

FIG. 14. Similar to Fig. 13, except that here it is V that varies. Notice the dip as V increases, just as in Fig. 13 for S.

to another part, as shown in Figs. 6 and 8. This is a rather peculiar feature of the specfic problem here, and as far as we know has not appeared before in any problem of a related type. The split-off states have a bound electron-hole character. In branch A they have a mixed symmetry $\psi^A(0)=0$, and $\psi^A(r)=+\psi^A(-r)$, whereas in branch B they have a mixed symmetry $\psi^B(0)\neq 0$, $\psi^B(r)=-\psi^B(-r)$.[14] The origin of this was discussed briefly at the end of Sec. 3. The states of lowest energy of branch B form a spin-wave spectrum. The other split-off states in branches A and B are excitons.

The exciton states cling rather closely to the band and, for the signs of the parameters we have chosen, lie just under the band. They may appear both in branch A and in branch B. In branch A they appear provided

$$|2V\sin K|<|J^{(z)}|\,, \quad \text{branch } A \tag{8.1}$$

and have energy [see Eq. (4.7)]

$$E=E_0-\tfrac{3}{2}J^{(z)}+V-8V^2|J^{(z)}|^{-1}\sin^2 K\,, \quad \text{branch } A\,. \tag{8.2}$$

The condition in Eq. (8.1) may be satisfied for some K but not others. (If $J^{(z)}=0$, it can *never* be satisfied.) Thus there may be a cutoff of the exciton branch, as actually shown in Fig. 10. The correlation function for the branch A exciton is [see Eq. (4.7)]

$$B_0=0, \quad |B_r|^2=(16V^2J^{(z)-2}\sin^2 K)^r, \quad \text{branch } A \tag{8.3}$$

where $|B_r|^2$ is the probability of finding the electron-hole separated by a distance r. Once beyond $r=0$ the probability $|B_r|^2$ decreases exponentially with r, indicating a true bound-state character. Notice that the exciton state also has an energy gap $\sim U$ from the ground state.

A similar kind of exciton state will also occur in branch B provided $\alpha_2>-1$ (see Sec. 5), which means provided [see case (3) below Eq. (5.8)]

$$|J^{(z)}|>\left|2V\sin K\frac{\eta}{\eta+4V\sin K}\right|\approx|2V\sin K|\,, \quad \text{branch } B\,. \tag{8.4}$$

This condition is very similar to Eq. (8.1) for the branch A exciton, and there can be a cutoff in the spectrum here also. The energy is more difficult to determine, but it is one of the solutions of a third-order algebraic equation, Eq. (5.7) which we shall not write down. It can be seen that the energy is of order U greater than the F-eigenstate energy. The correlation function for the state is

$$|B_r|^2=|B^0|^2[\alpha_I\pm(\alpha_I^2-1)^{1/2}]^r, \quad \alpha<-1, \quad \alpha>1, \quad \text{branch } B \tag{8.5}$$

where α_I is the intermediate root of Eq. (5.7). Once again there is an exponential decay for the probability of finding the electron near the hole.

Finally there is a generalized spin-wave state, obtained as the largest (in magnitude) root of Eq. (5.7).

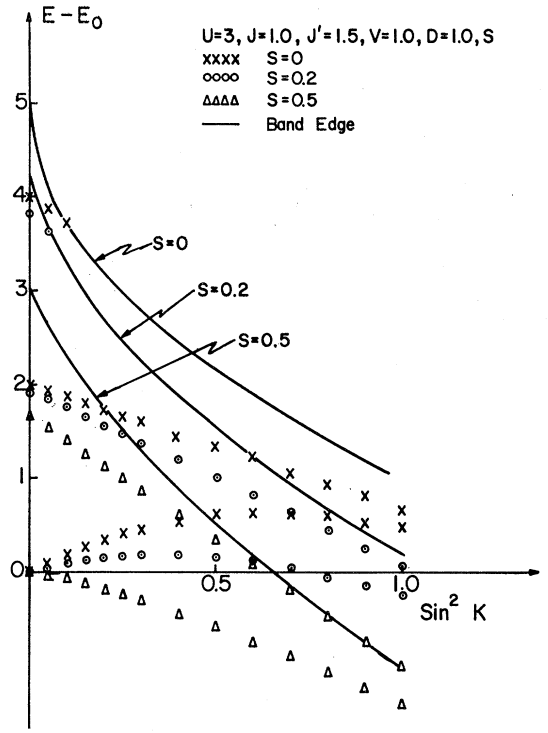

FIG. 15. This figure has the same description as Fig. 13, but with relatively smaller U. One can see from this figure how the spin wave and exciton spectrum can easily go below E_0 at the far end of the spectrum as S increases. This is discussed at the end of Sec. 8.

There are no conditions on this excitation: It always occurs. Its energy is approximately[18]

$$E_s=E_0+(-2J^{(z)}+2J^{(xy)}\cos 2K)-\frac{8V^2\sin^2 K}{U-2J^{(xy)}\cos 2K+\frac{1}{2}J^{(z)}}\,, \quad \text{spin wave} \tag{8.6}$$

and when $V=0$ it is clear that the energy is of the spin-wave form.

We see that the spin-wave states and the center of band are separated by a gap of magnitude $U+2J$. This, for large U, ensures the stability of the spin-wave states even for small $J^{(z)}$. But if U is kept fixed and $|J^{(z)}|$ increases the "exciton" spectrum in branch A comes down and may eventually overlap with the spin-wave states.

The final question to raise is the problem of stability of the ferromagnetic eigenstate. We can see from Eq. (8.6) that when V increases, the V^2-dependent negative term in the (E_s-E_0) expresison may overcome the positive spin-wave term, and hence yields the result that the generalized spin-wave states have energy lower than the ferromagnetic eigenstate energy, which implies that the latter is not stable. The criterion of having a stable ferromagnetic eigenstate would then be[18]

$$V<[\tfrac{1}{2}J(U-\tfrac{5}{2}J)]^{1/2}. \tag{8.7}$$

A criterion of this type was found by Slater[1] and by Paul.[3]

Also, the results of Sec. 7, when S, J', and D are included, indicate that the spin-wave branch may cross zero at $\sin K=1$ before the slope goes negative at $K=0$. This is then another criterion for the stability of the F state. In order to give some expression for this criterion, we can rewrite Eq. (6.14) in terms of E. It turns out to be of the form $AE^4+BE^3+CE^2+QE+R=0$. If $E=0$ at $\sin K=1$, then this equation can be satisfied only if $R=0$ (and conversely, this is a necessary condition). If for $\sin K=1$, E is slightly positive (i,e., ferromagnetism possible), then the criterion becomes

$$R/Q\leq 0, \quad \text{for stability.} \tag{8.8}$$

The expressions for Q and R are very long and tedious to derive. If S is set equal to zero, Eq. (6.14) can be separated into two branches A and B again. For branch B we find

$$R=64\{2V^2(2V^2+2J^2-Ja-2Jx)+J^2(a+x)\}, \tag{8.9}$$

$$Q=32\{Jx(a+x+2J)-V^2(a+2x)\}, \tag{8.10}$$

where

$$a=U+2J,$$
$$x=-\tfrac{1}{2}J-J'+D.$$

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APPENDIX: TURN-UPS AND TURN-OVERS

The object of this Appendix is to prove that the minimum of the turn-up and the maximum of the turn-over portions of the $G(E')$ curves of Figs. 6 and 8 lie above the value 1. The proof starts from Eq. (5.4):

$$\begin{aligned} G(E')&=g(\alpha)S(\alpha)-2x(\alpha-y), \\ S(\alpha)&=N^{-1}E(\alpha-\sin k)^{-1}. \end{aligned} \tag{A1}$$

Let there be zeros of $g(\alpha)$ at α_1, α_2. Then the statement is certainly true *at* these zeroes. For at $\alpha=\alpha_1$ $(i=1, 2)$

$$G(E_1')=2x(\alpha_i-y). \tag{A2}$$

Using Eqs. (5.6) this gives

$$G(E_i')=xy\left[1\pm\left(1-\frac{2}{xy}\right)^{1/2}\right], \quad i=1, 2 \tag{A3}$$

and it is easy to prove that

$$G(E_i')>1 \tag{A4}$$

using the fact that $z\equiv 2/xy$ must be <1 in order for the root to be real [see Eq. (5.6)].

It still remains to be proved for the root α_2 which lies in the interval $[\sin k_0, \sin(k_0+\Delta)]$, say, where $\Delta=2\pi/N$, that $G(E')$ lies above 1 in this entire interval [i.e., the minimum of $G(E')$ does not necessarily lie at α_2].

First of all, the variation of the term $2x(\alpha-y)$ in this interval is of order $1/N$ and this term may be regarded as being a finite value above 1 in the entire interval.

It must then be shown that the other term, gS, is either of order $1/N$ in the entire interval and hence does not affect the value obtained at α_i or else is positive. We know that S goes from $+\infty$ to $-\infty$ in the interval, and has a zero at, say, α_0 in the interval. Further, α_2 is also in this interval. Without loss of generality, let α_0 be to the left of α_2. Thus gS is positive on the edges of the interval, i.e., to the right of α_2 and to the left of α_0, in the interval. In these edge regions bounding the interval, therefore, the term gS increases $G(E')$ positively, and $G(E')$ therefore remains above 1. But for $\alpha_0<\alpha<\alpha_2$, gS is negative, and can conceivably cause $G(E')$ to drop below 1. However in this region gS is of order $1/N$.

To see this, divide S into two parts S_a+S_b, where S_a contains a few terms around k_0, and S_b contains the rest. S_b can be evaluated by conversion to an integral,

$$S_b=\frac{1}{2\pi}\left[\int_{-\pi}^{k_0-\delta}+\int_{k_0+\delta}^{\pi}\right]\frac{dk}{\alpha-\sin k}\cong 0(\delta), \quad \delta\ll 1 \tag{A5}$$

where δ represents an interval around k_0. This integral is finite (is zero, in fact, if $\delta=0$), and gS_b is negligible since g is of order $1/N$.

The other part S_a, containing just a few terms, can be estimated and it is also finite, since we are not close to the asymptotic region. Once again multiplication by g gives a contribution of order $1/N$, and the assertion is proved.

Of course the obverse of the assertion of this Appendix is that when a state is lost from the band, it must occur below (or above) the band. We do not include it here but a quite rigorous proof can be made starting from Eq. (5.7) showing that roots do appear below (or above) the band whenever states are lost in the band. Rather than include the mathematical details, we have provided the figures, which show more vividly how these roots transfer from in to out of the band as the roots of $g(\alpha)$ move into the band.