by Seifert (Ref. 2), that a_0 and c_0 of his unit cell are one and one-third of the respective values given by Seifert.
[10]E. F. Bertaut, Acta Cryst. A24, 217 (1968).
[11]G. Shirane, Acta Cryst. 12, 282 (1959).
[12]H. Shaked and S. Shtrikman, Solid State Commun. 6, 425 (1968).
[13]E. A. Turov, *Physical Properties of Magnetically Ordered Crystals* (Academic, New York, 1965), p. 134.

PHYSICAL REVIEW B VOLUME 3, NUMBER 3 1 FEBRUARY 1971

Ferromagnetic Spin Excitations in a One-Band Metallic Loop, the Case of Long-Range Interactions

J. Chen and M. Bailyn
Department of Physics, Northwestern University, Evanston, Illinois* 60201
(Received 17 June 1970)

We extend the previous treatment of one-band spin excitations to include an arbitrary band term and a long-range two-body interaction. The system still consists of N electrons in a periodic loop lattice with N sites. It is found that the number of bound states depends on the range of the effective two-body interaction, and that the distribution in energy scale of these bound states depends on the spatial variation of the two-body interaction strength.

In a previous paper,[1] we considered a system of N electrons in a periodic loop potential which has N lattice sites. A one-band Hamiltonian containing a nearest-neighbor interaction was considered, and the one-spin-flip spectra relative to a saturated ferromagnetic eigenstate were calculated exactly.

It was found that the characteristic terms contributing to the spin-wave spectrum are the band term, the correlation term ($\sim n_i n_{i'}$), and the intersite exchange term. In the present paper we shall extend the treatment to arbitrary band structure and to include more than nearest-neighbor terms for the two-body interaction. The explicit form of the Hamiltonian is as follows[2]:

$$H = H_b + H_c + H_{\mathrm{ex}} , \tag{1}$$

where

$$H_b = \sum_k \sum_\sigma \mathcal{E}_k C^\dagger_{k,\sigma} C_{k,\sigma} , \tag{2}$$

$$H_c = U_0 \sum_{i=1}^{N} n_{i,+} n_{i,-} + \sum_{i=1}^{N} \sum_{l=1}^{N-1} U_l (n_{i,+} + n_{i,-}) \times (n_{i+l,+} + n_{i+l,-}), \tag{3}$$

$$H_{\mathrm{ex}} = -\sum_{i=1}^{N} \sum_{l=1}^{N-1} J_l (C^\dagger_{i,+} C_{i,-} C^\dagger_{i+l,-} C_{i+l,+} + \mathrm{H.c.}) - \sum_{i=1}^{N} \sum_{l=1}^{N-1} \frac{J_l}{2} (n_{i,+} - n_{i,-})(n_{i+l,+} - n_{i+l,-}), \tag{4}$$

where $C^\dagger_{i,\sigma}$, $C_{i,\sigma}$, $n_{i,\sigma}$, are, respectively, the creation, anihilation, and number operator of the ith Wannier orbital with spin index σ, and $C^\dagger_{k,\sigma}$, $C_{k,\sigma}$ are the Bloch operators with wave vector k, and where

$$U_l = U_{-l} = U_{N+l} , \tag{5}$$

$$J_l = J_{-l} = J_{N+l} .$$

The Wannier and Bloch operators are related by

$$C_{k,\sigma} = N^{-1/2} \sum_{l=1}^{N} e^{ikl} C_{l,\sigma} ,$$

$$k = \frac{2\pi}{N} n , \quad n = 0, 1, 2, \ldots, (N-1). \tag{6}$$

The band Hamiltonian can be rewritten in terms of Wannier operators as

$$H_b = \sum_{l,m} \sum_\sigma V(l-m) C^\dagger_{l,\sigma} C_{m,\sigma} , \tag{2'}$$

where

$$V(l) = N^{-1} \sum_k e^{ikl} \mathcal{E}_k . \tag{7}$$

Let $|\phi_0\rangle$ be the state with all Wannier sites occupied by down-spin electrons and with no up-spin electrons, then $|\phi_0\rangle$ is an eigenstate of the Hamiltonian H with eigenvalue

$$E_0 \equiv \langle \phi_0 | H | \phi_0 \rangle = \sum_k \mathcal{E}_k + N \sum_{l=1}^{N-1} (U_l - \tfrac{1}{2} J_l). \tag{8}$$

Since the Hamiltonian commutes with the total spin of the system, the simplest stable excitation will be where $N-1$ electrons have down-spin, and one electron has up-spin. Let us consider the one-spin-flip states

$$\Psi_{f,g} \equiv C^\dagger_{f,+} C_{g,-} | \phi_0 \rangle , \tag{9}$$

and solve the Schrödinger's equation in the subspace spanned by $\{\Psi_{f,g}\}$,

$$H\Psi = E\Psi , \tag{10}$$

where

$$\Psi = \sum_{f,g} A_{f,g} \Psi_{f,g} , \tag{11}$$

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

$$A_{f+N,g}=A_{f,g}\ ,\qquad A_{f,g+N}=A_{f,g}\ . \tag{12}$$

To solve the eigenvalue problem, we first calculated $H\Psi_{f,g}$, and substitute the result into Eq. (10), then shift indexes under the summation sign noticing that the $\Psi_{f,g}$'s are all linearly independent; we then arrive at

$$\sum_l [V(f-l)A_{l,g}-V(l-g)A_{f,l}]-U_0\delta_{f,g}A_{f,g} -\sum_{l=1}^{N-1} J_l\delta_{f,g}(A_{f-l,g-l}+A_{f+l,g+l}) -\sum_{l=1}^{N-1}(U_l+\tfrac{1}{2}J_l)(\delta_{f,g+l}+\delta_{f,g-l})A_{f,g}=E'A_{f,g}, \tag{13}$$

where

$$E'\equiv E-E_0-\left(U_0+\sum_{l=1}^{N-1}2J_l\right). \tag{14}$$

To solve Eq. (13), let us try solutions of the following form:

$$A_{f,g}=e^{iK(f+g)}B_{f-g},\qquad K=\frac{\pi}{N}n\ ,\ n=0,1,2,\ldots,\ (N-1). \tag{15}$$

Substituting Eq. (15) into Eq. (13) and simplifying, we have[3]

$$\sum_{l=1}^{N}V(l)e^{iKl}\,(B_{r+l}-B_{r-l})-\tilde{U}_rB_r=E'B_r, \tag{16}$$

where

$$r\equiv f-g,\quad r=1,2,\ldots,N \tag{17}$$

$$\tilde{U}_0\equiv U_0+\sum_{l=1}^{N-1}2J_l\cos 2Kl, \tag{18}$$

$$\tilde{U}_r\equiv(U_r+\tfrac{1}{2}J_r),\quad r\geq 1. \tag{19}$$

We take the Fourier transform of B_r:

$$b_k=\sum_{r=1}^{N}e^{ikr}B_r\ , \tag{20}$$

or

$$B_r=N^{-1}\textstyle\sum_k e^{-ikr}b_k\ . \tag{21}$$

If we multiply Eq. (16) by e^{ikr} and sum over all r, we then have

$$b_k=\sum_l\frac{e^{ikl}}{E_k(K)-E'}\tilde{U}_lB_l\ , \tag{22}$$

where

$$E_k(K)\equiv\mathcal{E}_{k-K}-\mathcal{E}_{k+K}\ . \tag{23}$$

If we multiply Eq. (22) by e^{-ikr} and sum over k, we obtain

$$B_r=\textstyle\sum_l G(r,l)\tilde{U}_lB_l,\quad r=0,1,2,\ldots\ (N-1) \tag{24}$$

where

$$G(r,k)\equiv N^{-1}\sum_k\frac{e^{-ik(r-l)}}{E_k(K)-E'}\ . \tag{25}$$

Equation (24) is of the form of an integral equation of the Fredholm type; for given $\tilde{U}_l$ and $\mathcal{E}_k$, there are standard approximation procedures to find its solutions. However, for a short-range effective two-body interaction, i.e., if $\tilde{U}_l=0$ for $|l|>M$, where M is a positive integer representing the range of interaction, one can obtain a $(2M+1)\times(2M+1)$ determinantal equation by letting $r=0,\pm1,\ldots,\pm M$ in Eq. (24).

A special case, the case of $M=1$, has been solved in detail in Ref. 1, where the structure of the energy eigenstates are explicitly shown.[4] There are both continuum states and bound states which lie below the continuum. The structure of the continuum states is indicated by the energy denominators in the summations over k, and it was shown how bound states are formed by dropping out of the continuum.[5] One would expect that this feature of the formation of continuum and bound states remains unchanged for Hamiltonians involving more than nearest-neighbor interactions except, of course, that the number and distribution (in energy scale) of the possible bound states depend on the range and spatial variation of the effective two-body interaction. To see this point more explicitly, let us look at the $K=0$ case from Eq. (16):

$$(E'+\tilde{U}_r)\,B_r=0,\quad r=0,1,2,\ldots\ (N-1). \tag{16'}$$

The equations no longer couple different B_r's, and the solutions are immediate. They fall into three groups of ascending energies.

(I) One spin-wave state:

$$E'+\tilde{U}_0=0,\ \text{i.e.},\ E=E_0,\ \text{and}\ \begin{cases}B_0\neq 0\\ B_{r'}=0,\ r'\neq 0.\end{cases} \tag{26}$$

(II) $2M$ exciton states degenerate in pairs:

$$E'+\tilde{U}_r=0,\ \text{i.e.},\ E_r=E_0+\left(U_0+\sum_{l=1}^{M}4J_l\right)-\tilde{U}_r\ ,$$

$$\text{and}\ \begin{cases}B_r\ \text{and/or}\ B_{-r}\neq 0\\ B_{r'}=0,\ r'\neq r,-r,\quad r=\pm1,\pm2,\ldots,\pm M.\end{cases} \tag{27}$$

(III) $N-2M-1$ degenerate continuum states:

$$E'+\tilde{U}_r=0,\ \text{i.e.},\ E=E_0+\sum_{l=1}^{M}4J_l+U_0\ ,$$

$$\text{and}\ \begin{cases}B_l=0,\ l=0,\pm1,\ldots\pm M\\ \text{the rest arbitrary}\\ r=\pm(M+1),\pm(M+2),\ldots,\pm(N-1)/2.\end{cases} \tag{28}$$

If $M=\frac{1}{2}(N-1)$ (for N odd), then the interaction ranges over the whole loop, in which case there is

no well-defined continuum. Notice the physical significance of the B_r's of the continuum states. The fact that $B_r = 0$ for $r \leq M$ means that the electron and hole are "out of range" of their mutual effective interaction. (This is analogous to the continuum states of, say, a hydrogen atom.)

By the same token, notice the physical significance of the B_r's for the exciton states. The fact that $B_{\pm r} \neq 0$, and all the other B_l's $= 0$, means that the electron-hole distance is fixed at r atom distances. For the spin-wave state, the electron is fixed to be over the hole!

To look at the behavior of the bound states in the neighborhood of $K = 0$, a first approximation is to let $G(r, l) = 0$ for $l \neq r$ [6]; under this approximation, Eq. (24) becomes

$$\left(1 - N^{-1}\sum_k \frac{\tilde{U}_r}{E_k(K) - E^r}\right) B_r = 0, \qquad r = 0, \pm 1, \ldots, \pm M. \tag{29}$$

For bound states, the summation over k can be replaced by an integral using the correspondence $N^{-1}\sum_k \to (2\pi)^{-1}\int_{-\pi}^{\pi} dk$. Using only the nearest-neighbor terms in H_b, i.e., $\mathcal{E}_k = V_0 + 2V\cos k$, the solutions of Eq. (29) are found to be

$$E_r^{(k)} - E_0 = \left(U_0 + \sum_{l=1}^{M} 4J_l\right) - (U_r^2 + 16V^2\sin^2 K)^{1/2}, \qquad r = 0, \pm 1, \ldots, \pm M. \tag{30}$$

A schematic diagram of the continuum states and the bound states are shown in Fig. 1 (using $\mathcal{E}_k = V_0 + 2V\cos k$). It is, of course, understood that

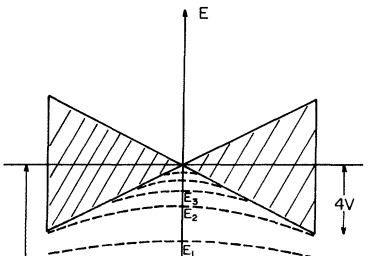

FIG. 1. Schemetic diagram showing continuum and bound states. The concave-upward curve that hits the $E = E_0$ level at $K = 0$ is the spin-wave spectrum. The concave-downward dotted lines are the exciton spectra, and the shaded region represents the continuum. The energies of $K = 0$ are known explicitly: $E_1 = E_0 + E_g - \tilde{U}_1$, $E_2 = E_0 + E_g - \tilde{U}_2$, etc. [see Eq. (27)].

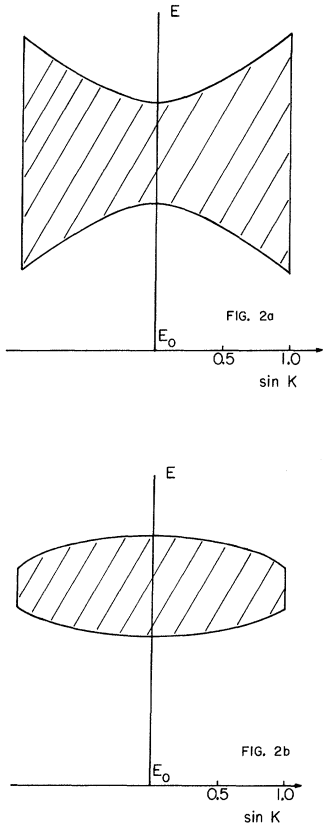

FIG. 2. Effect of the semihopping term on the structure of the continuum. The continua in (a) and (b) are obtained by letting $S = \frac{3}{4}V$ and $-\frac{3}{4}V$, respectively.

the bound states will eventually merge into the continuum when their spectra are "caught up" by the lower edge of the band.

As an example of showing possible long-range effects, let us consider another extreme case, for which $U_l = U_\infty = \text{const}$, $l = 1, 2, \ldots, (N-1)$, and $J_l = 0$ except for $l = \pm 1$. Under these conditions, Eq. (22) becomes

$$b_k = \frac{(\tilde{U}_0 - U_\infty)B_0 + J_1(e^{ik}B_1 + e^{-ik}B_{-1}) + U_\infty b_k}{E_k(K) - E'} \tag{22'}$$

or

$$b_k = \frac{(\tilde{U}_0 - U_\infty)B_0 + J_1(e^{ik}B_1 + e^{-ik}B_{-1})}{E_k(K) - E''}, \tag{31}$$

where

$$E'' = E' + U_\infty . \tag{32}$$

Equation (31) has the form as if there were only nearest-neighbor exchange interaction and on-site correlation [compare with Eq. (22)]. The solutions to Eq. (31) were given in detail in Ref. 1, and it was shown that there are at most three bound states. The effect of a constant long-range correlation is just to reduce the gap between all the continuum

states and the ferromagnetic eigenstate E_0 by an amount U_∞, but the continuum remains a continuum! To remove the degeneracy of the continuum at $K=0$, we need a potential $\tilde{U}_l$ which differentiates between various electron-hole distances. As we have seen before, this degeneracy was only partially removed when the interaction is short ranged; short-range interaction means that $\tilde{U}_l$ does not differentiate between various electron-hole distances when these distances go beyond a certain limit.

Let us finally discuss some of the effects on continuum and bound states when the semihopping[2] term H_s is introduced. For simplicity, we shall consider only the nearest-neighbor terms for both the band and semihopping terms:

$$\begin{aligned} H_s = S \sum_{i=1}^{N} [& C^\dagger_{i,+} C_{i+1,+} (n_{i,-} + n_{i+1,-}) \\ & + C^\dagger_{i,+} C_{i-1,+} (n_{i,-} + n_{i-1,-}) \\ & + C^\dagger_{i,-} C_{i+1,-} (n_{i,+} + n_{i+1,+}) \\ & + C^\dagger_{i,-} C_{i-1,-} (n_{i,+} + n_{i-1,+})] . \end{aligned} \tag{33}$$

Solving the energy eigenvalue equation as before, the equation corresponding to Eq. (22) would then be of the form

$$b_k = \sum_l \frac{\rho_l(k, K) B_l}{\xi \sin(k+\varphi) - E'} , \tag{34}$$

where

$$\xi \equiv 4[(V+S)^2 \sin^2 K + S^2 \cos^2 K]^{1/2} , \tag{35}$$

$$\sin\varphi \equiv S \cos K / \xi , \tag{36}$$

and where $\rho_l(k, K)$'s are functions of S, U_l, etc., which can be easily found.

Since the energy denominators indicate the continuum states, we see that the semihopping term actually alters the structure of the continuum states. It should be noted that, at $K=0$, $\xi = 4S \neq 0$. This means that the band width at the $K=0$ point is nonzero, and that the formerly degenerate continuum states at $K=0$ are dispersed into a band of width $8S$. The shape of the band actually depends on the magnitudes and signs of V and S.[7] Two different types of continuum are illustrated in Fig. 2. The bound-state spectra are also perturbed when H_s is introduced, and they exist only below the continuum.[1]

---

*Research supported in part by the National Science Foundation under Grant No. GP 11054, and by the Advanced Research Project Agency of the Department of Defense through the Material Research Center at Northwestern University.

[1] J. Chen and M. Bailyn, Phys. Rev. B 1, 3030 (1970).

[2] The Hamiltonian in Eq. (1) is not of the most general form. The semihopping and double-hopping terms (H_S and H_D) discussed in Ref. 1 are left out. It should be remembered that the only term which has a true long-range character is U_l, since the J_l's, S_l's, and D_l's (see Ref. 1) all involve exchange or overlap integrals. These cause them to get small as l gets large, much faster than does U_l. Therefore, the neglect of the long-range part of J_l, S_l, D_l, etc., is a reasonable first approximation. At the end of the present paper some of the effects of S_l for $l=1$ are discussed. Also left out are the 3-site and 4-site terms always present in the second-quantized two-body interaction Hamiltonian. For a general classification of terms see, for example, M. Bailyn, Advan. Phys. 15, 179 (1966), Sec. 1.3.3.

[3] Notice that $\tilde{U}_r = \sum_l \tilde{U}_l \delta_{r,l}$.

[4] The electron-hole problem with nearest-neighbor interactions treated in Ref. 1 is quite close in mathematical structure to the two-magnon problem discussed by M. Wortis, Phys. Rev. 132, 85 (1963), and others.

[5] The figures and corresponding discussions in Ref. 1 give the details.

[6] The justification of this approximation lies in the fact that for bound states near $K=0$, $|E'| \gg |E_k(K)|$; the $G(r, l)$ function for $r \neq l$ is then a sum over k of $e^{ik(r-l)}$ divided by a slowly varying denominator. For nearest-neighbor hopping, $G(r, l) \sim [\alpha - (\alpha^2 - 1)^{1/2}]^{|r-l|}$, where $\alpha = |E'/(4V \sin K)|$. Thus $G(r, l)$ decreases exponentially as $|r-l|$ increases.

[7] S is usually positive, but there is no reason why V should have the same sign.