Ferromagnetic spin waves in quasiperiodic superlattices

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A formulation of ferromagnetic spin waves in quasiperiodic superlattices at low temperature is given. The spectra, wave functions, and some related physical quantities of these systems are discussed and specified extended states are found. Numerical results are carried out to exhibit the effect of quasiperiodicity on these systems.

I. INTRODUCTION

Since the discovery of icosahedral point-group symmetry in Al-Mn alloys,[1] a new class of ordered structures (quasicrystals) with quasiperiodic translational order have been extensively studied.[2] These structures are intermediate between the completely periodic perfect crystals and the random or disordered amorphous solids. The electronic and vibrational properties of these structures have been investigated in considerable depth both numerically and analytically in one dimension (1D) (Ref. 3) and numerically in higher dimensions.[4] Many interesting features such as exotic band structures and critical wave functions have been found. In this paper, we start to study another kind of low-temperature excitation, spin waves, in a new kind of material, a quasiperiodic superlattice, which was made in laboratory originally for semiconductor studies.[5] In the following, we first give the formulation of this problem in Sec. II, and then discuss the spectra, wave functions, and some related physical quantities of this new system in Secs. III, IV, and V, respectively.

II. FORMULATION

Now consider a quasiperiodic superlattice consisting of two kinds of single atomic planes A and B, arranged in the form of Fibonacci sequence[3] described by the recursive relation $S_{j+1}=\{S_j,S_{j-1}\}$ for $j\geq 1$ with $S_0=\{A\}$ and $S_1=\{AB\}$. This structure we consider is still periodic along the direction parallel to the atomic planes (layers) but quasiperiodic perpendicular to them. The Heisenberg Hamiltonian for the present system can be written as

$$H=-\sum_{m,n}\sum_{i,j}J(n,i;m,j)\hat{\mathbf{s}}(n,i)\cdot\hat{\mathbf{s}}(m,j)\ , \qquad (2.1)$$

where m,n are indices of atomic planes and i,j sites in atomic planes n and m, respectively. The interaction constant $J(n,i;m,j)$ is nonzero only when the sites are nearest neighbor and take the following value:

$$J(m,j;n,i)=\begin{cases} J_A & \text{for both sites} \in A \\ J_B & \text{for both sites} \in B \\ J_{AB} & \text{for one site} \in A \text{ and the other} \in B\ . \end{cases} \qquad (2.2)$$

In this paper, we only consider the ferromagnetic case with $J(m,j;n,i)>0$ and $\hat{\mathbf{s}}(n,i)\cdot\hat{\mathbf{s}}(n,i)=s(s+1)$ for all sites.

The ground state of the system considered is, like the periodic system, all spin parallel. Now let us consider the excitation of this system at low temperature. We first apply to H the Holstein-Primakoff transformation[6] and only take quadratic terms in H, then we have

$$H=H_0+s\sum_{n,m}\sum_{i,j}J(n,i;m,j)[a^{\dagger}(n,i)a(n,i)+a^{\dagger}(m,j)a(m,j)]-s\sum_{n,m}\sum_{i,j}J(n,i;m,j)[a^{\dagger}(n,i)a(m,j)+a(n,i)a^{\dagger}(m,j)]\ , \qquad (2.3)$$

where H_0 is the ground-state energy. In order to diagonalize Hamiltonian (2.3), we take advantage of the periodicity in the layers and take the corresponding Fourier transformation. We then introduce the following further transformation:

$$\begin{aligned} c_{pk}&=(1/\sqrt{N})\sum_n f_p(n)b(n,k)\ ,\\ c_{pk}^{\dagger}&=(1/\sqrt{N})\sum_n f_p^*(n)b^{\dagger}(n,k)\ , \end{aligned} \qquad (2.4)$$

where N is the number of total atomic planes, k the wave vector parallel to the layers, and $f_p(n)$ is a wave function to be determined by

$$(J_{n,n+1}+J_{n,n-1}+J_{n,n})f_p(n)-J_{n,n-1}f_p(n-1)-J_{n,n+1}f_p(n+1)=w_{pk}f_p(n)/2s \qquad (2.5)$$

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for all n. Here $J_{n,m}$, $b(n,k)$, and $b^{\dagger}(n,k)$ are the Fourier partition of $J(n,i;m,j)$, $a(n,i)$, and $a^{\dagger}(n,i)$, respectively. For layers of simple cubic structure normal to the (001) direction, we have

$$J_{n,n}=[4-2\cos(k_x d)-2\cos(k_y d)] \times J(n,i;n,i\pm 1)\equiv r_k J_n . \quad (2.6)$$

With the above transformations, the Hamiltonian (2.3) is finally diagonalized in the form

$$H=H_0+\sum_k \sum_p w_{pk} c_{pk}^{\dagger} c_{pk} , \quad (2.7)$$

where w_{pk} is the excitation energy of the spin waves in the quasiperiodic superlattice at low temperature, which can be obtained from the eigenvalues in the solution of Eq. (2.5). We will study it in the next section.

III. SPECTRA

Now we begin to study the spectra of spin waves of a simple cubic structure for which Eq. (2.6) is valid. Other cases can be treated similarly. Since Eq. (2.5) is similar to 1D quasiperiodic models, we can use the method of Ref. 3 to calculate the structure of the energy band. In the present case, the related transfer matrix[3] of block S_j, denoted by M_j, satisfies the following recursive relation:

$$M_j=M_{j-1}M_{j-2} \text{ for } j>2 ,$$

with

$$M_1=T_{ABA}T_{BAB} \text{ and } M_2=T_{ABA}T_{BAA}T_{AAB} , \quad (3.1)$$

where

$$T_{BAB}=\begin{bmatrix} 2-x_A & -1 \\ 1 & 0 \end{bmatrix}, \quad T_{BAA}=\begin{bmatrix} 1+(1-x_A)/\lambda & -1/\lambda \\ 1 & 0 \end{bmatrix},$$

$$T_{ABA}=\begin{bmatrix} 2-X_B & -1 \\ 1 & 0 \end{bmatrix}, \quad T_{AAB}=\begin{bmatrix} 1+\lambda-x_A & -\lambda \\ 1 & 0 \end{bmatrix},$$

and

$$x_A\equiv w-r_k\lambda, \quad x_B\equiv w-r_k\beta\lambda, \quad \beta\equiv J_B/J_A , \quad w\equiv w_{pk}/2sJ_{AB}, \quad \lambda\equiv J_A/J_{AB} . \quad (3.2)$$

With the above expressions and the periodic approximation,[3] we calculated the allowed energy of the system for some values of j, the results are shown in Figs. 1 and 2. We see from Fig. 1 that the number of subbands at step j is equal to the Fibonacci number[3] F_j (with $F_0=1$ and $F_1=2$) for $j>2$ and related to the value of r_k for $j\leq 2$. The band structure in Fig. 1 is different from that of a transfer-phonon model of 1D quasicrystals[3] as well as that of an on site electronic model[3] and has nonuniform scaling depending on values of w in a more complicated way. The dependence of the band structure on parameter r_k is shown in Fig. 2. As r_k increases in value, the bandwidths become narrower, the gaps are enlarged, and energy bands themselves are shifting upward to a degree depending also on the value of β.

The integral density of state $I(w)$ for the spin waves of the quasiperiodic superlattice in the periodic approximation is expressed by

$$I(w)\cong I_j(w)=\sum_k I_k^j(w) ,$$

$$I_k^j(w)=\int_0^w dw'\,\Theta(2-|x_j(w')|)\,|x_j'(w')|/(2\pi\{1-[x_j(w')/2]^2\}^{1/2}) ,$$

where

$$\Theta(x)=\begin{cases} 1, & x>0 \\ 0, & x<0 \end{cases}$$

$$x_j'(w')\equiv \left.\frac{\partial x_j(w)}{\partial w}\right|_{w=w} ,$$

and

$$x_j(w')\equiv \mathrm{Tr} M_j . \quad (3.3)$$

When $j\to\infty$ in Fig. 1, we expect to observe the "Cantor-set" spectra for fixed k, and the sufficient conditions for the value of w with given k to lie in the gaps of energy bands at an infinite value of j', there exists a value of l satisfying

$$|x_{l-2}(w)|\leq 2, \quad |x_{l-1}(w)|\geq 2, \quad \text{and} \quad |x_l(w)|\geq 2 , \quad (3.4)$$

since $x_j(w)$ is then unbounded.[3]

IV. WAVE FUNCTION

We now turn to study the wave function of the spin waves in the infinite quasiperiodic superlattice.[7] Since

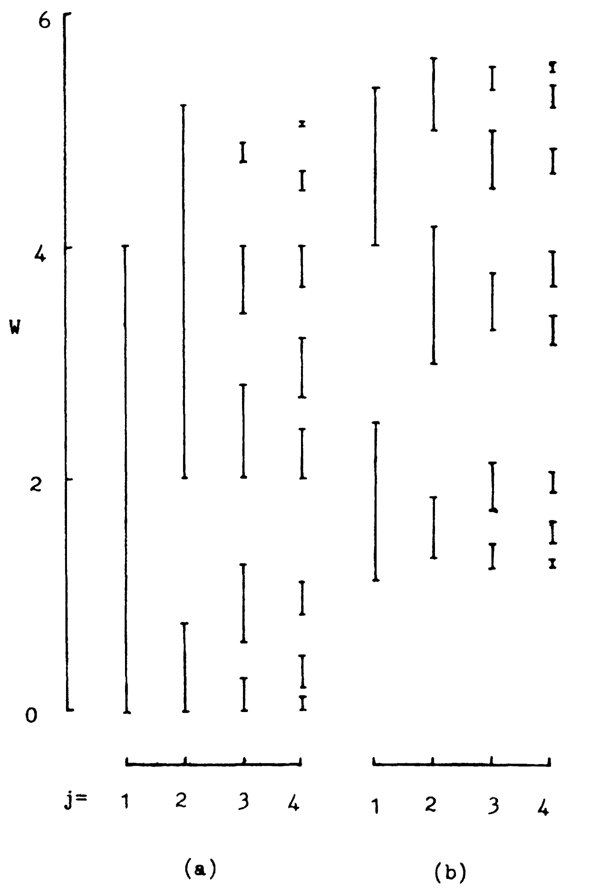

FIG. 1. The allowed energy w for $j=1$, 2, 3, 4 and 5 with (a) $\lambda=2$, $r_k=0$, and $\beta=\frac{1}{4}$; (b) $\lambda=1$, $r_k=2$, and $\beta=\frac{1}{4}$.

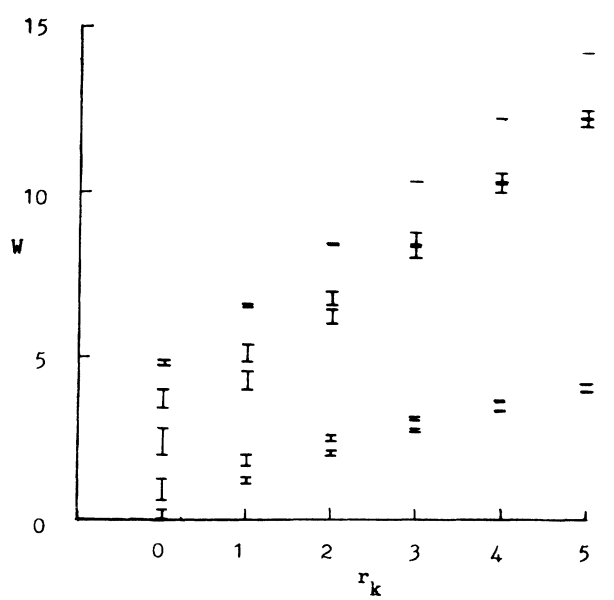

FIG. 2. Variation of band structure with parameter $r_k \equiv 4-2\cos(k_x d)-2\cos(k_y d)$ for $j=3$, $\lambda=2$, and $\beta=\frac{1}{4}$.

the system retains periodicity along the direction parallel to the atomic planes, the spin waves must be extended in this direction. The study of the properties of the spin waves along the direction perpendicular to the atomic planes is reduced to the analysis of Eq. (2.5) resulting from a 1D problem. Recently, Kohmoto[3] and Ostlund *et al.*[8] have confirmed that the wave functions of their 1D quasiperiodic model are always critical, namely, they are either self-similar or chaotic. Since Eq. (2.5) is an eigenvalue equation of a generalized 1D Fibonacci lattice system, the wave functions of Eq. (2.5) should be characterized by critical states. However, we will show in the following that some specified extended states, apart from the critical states, can also exist in the present quasiperiodic system.[9]

From relations (3.1) and (3.2) it is easy to see that if $x_A=x_B=2$, which is true when $w_{pk}^0=4sJ_{AB}$ under the condition $r_k=0$, then we have

$$M_1=\begin{bmatrix}-1 & 0\\ 0 & -1\end{bmatrix},\quad |\mathrm{Tr}M_2|=2|\lambda-1| \ . \tag{4.1}$$

That means that block S_1 is transparent for the wave with energy w_{pk}^0. Since the quasiperiodic system is constructed by two building blocks S_1 and S_2, or more generally by S_j and S_{j+1} for $j\geq 1$, then if w_{pk}^0 is also in the energy band of the regular system constructed by block S_2, that is $|\lambda-1|\leq 1$, the quasiperiodic system can have an extended state with energy w_{pk}^0. In general, if for some values of j the following conditions are satisfied for a value of w:

$$M_j=\pm\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix},\quad |\mathrm{Tr}M_{j+1}|\leq 2 \ , \tag{4.2}$$

there may exist an extended state with energy w in the quasiperiodic system. Since extended states play quite a different role from that of critical states in physical processes such as transport process, so the fact might be important that there exists some special extended states in quasiperiodic systems.

V. PHYSICAL QUANTITY

In order to manifest some effects of quasiperiodicity on physical quantities, we calculated the deviation of magnetization $\Delta M(T)\equiv s-M(T)/g\mu_B$ and the magnetic specific heat C_v for the quasiperiodic superlattice with a finite number of atomic planes F_{15} as well as a periodic superlattice constructed by successive repeating of building block AB. We see from our calculational results that quasiperiodicity decreased the value of C_v due to the increase of gaps in the quasiperiodic system, but the dependence of C_v on temperature $T^{3/2}$ appears not to be effected by quasiperiodicity at sufficiently low temperature, as shown in Fig. 3. Similar results are also obtained for $\Delta M(T)$. As the temperature increases, the discrepancy between the slopes of the two curves in Fig. 3, howev-

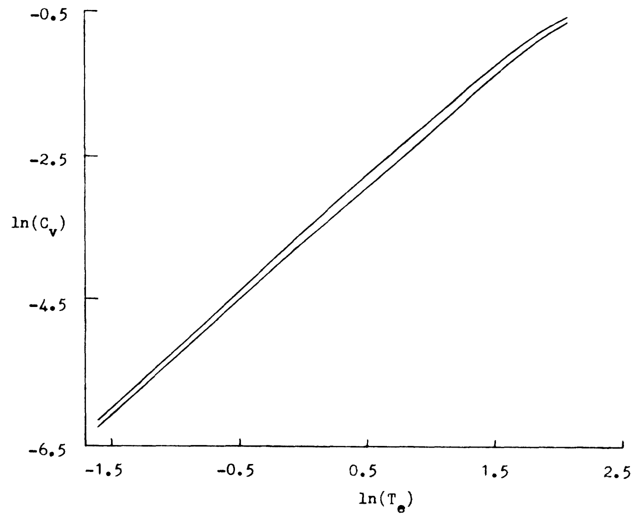

FIG. 3. Magnetic specific heat c_v vs temperature T_e for $\lambda=5$ and $\beta=1$. The upper curve stands for the periodic system and the lower for the quasiperiodic system.

er, becomes noticeable due to the effect of large gaps. For higher temperature, Eq. (2.3) is no longer valid, we will pursue the proper treatment for this case in our further study.

VI. SUMMARY

On the basis of our formulation of the problem of ferromagnetic spin waves in quasiperiodic superlattices at low temperature, we have discussed the spectra of spin waves and found some new global structures of energy bands different from that of a transfer-phonon model as well as an on-site electronic model of 1D quasicrystal systems. An expression for the integral density of states of the spin waves is given. The study of wave functions indicates that along the direction parallel to the atomic planes (or interfaces) the wave functions are extended, and in the direction perpendicular to the interfaces, in addition to critical states characterizing mainly the wave function, there can also exist some states which are extended in this direction. The numerical calculations carried out by us for the magnetization and the magnetic specific heat at low temperature exhibited the effect of quasiperiodicity on them. It appears that the $T^{3/2}$ law is good enough at sufficiently low temperature.

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[9]Recently, Kumar and Ananthakrishna [Phys. Rev. Lett. **59**, 1476 (1987)] have shown, in the study of electronic structures of quasiperiodic superlattices, that some extended states do exist in their systems when the number of layers per slab is larger than 1, that is, $N,M>1$ in their paper. Here we see that extended states may exist even for $M=N=1$ in the present similar system.