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Excitation Spectra of Linear Magnetic Chains*

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The restrictions on the excitation spectra of infinite linear magnetic chains due to the invariances of the Hamiltonian under time reversal and spin rotation have been studied by making use of the equivalence of a linear magnetic chain and a one-dimensional assembly of interacting Fermi particles. In particular, the spin-wave spectrum of an infinite antiferromagnetic chain is found to have a double periodicity of π in the wave vector, in agreement with the numerical result of des Cloizeaux and Pearson.

THE exact spin-wave spectrum of a linear antiferromagnetic chain of spin $\frac{1}{2}$ was calculated by des Cloizeaux and Pearson.[1] A striking feature of this spectrum for an infinite chain is its double periodicity of π in the wave vector, in addition to the periodicity of 2π as one expects from the translational symmetry of the chain. This is puzzling because one cannot expect the two-sublattice situations here as in the theories of Anderson and Kubo.[2] The purpose of this paper is to point out a simple connection between this double periodicity and the symmetry properties of the linear magnetic chain.

We consider a magnetic chain of spin $\frac{1}{2}$ coupled to the nearest neighbors having the following Hamiltonian:

$$H=\sum_{l=1}^{N}\left[\alpha(S_l^xS_{l+1}^x+S_l^yS_{l+1}^y)+\gamma S_l^zS_{l+1}^z\right],\qquad \mathbf{S}_{N+1}=\mathbf{S}_1. \quad (1)$$

We now express the spin operators in terms of Fermi particle operators c_l and $c_l^\dagger$ as follows[3]:

$$S_l^x=\tfrac{1}{2}(a_l^\dagger+a_l),\quad S_l^y=(1/2i)(a_l^\dagger-a_l),\quad S_l^z=a_l^\dagger a_l-\tfrac{1}{2}, \quad (2)$$

where

$$a_l=\exp\Big(-\pi i\sum_{j=1}^{l-1}c_j^\dagger c_j\Big)c_l,\quad a_l^\dagger=c_l^\dagger\exp\Big(\pi i\sum_{j=1}^{l-1}c_j^\dagger c_j\Big). \quad (3)$$

By neglecting the end effects, we require the transformed Hamiltonian to have a translational symmetry in the Fermi operators by imposing $c_{N+1}=c_1$, $c_{N+1}^\dagger=c_1^\dagger$ (c-cyclic problem[3]). Thus we are restricting ourselves to infinite chains.

The symmetry properties of this system have been discussed elsewhere[4]; there are two nontrivial symmetry operations which leave the Hamiltonian invariant besides the translation. They are the time-reversal K and the rotation of spins by 180° about the y axis R, namely,[4]

$$Kc_lK^{-1}=(-1)^lc_l^\dagger,\quad Kc_l^\dagger K^{-1}=(-1)^lc_l,\quad KiK^{-1}=-i; \quad (4)$$

$$Rc_lR^{-1}=(-1)^lc_l^\dagger,\quad Rc_l^\dagger R^{-1}=(-1)^lc_l,\quad RiR^{-1}=i. \quad (5)$$

By introducing the Fourier transforms of Fermi operators,

$$c_k=N^{-1/2}\textstyle\sum_l e^{-ikl}c_l,\quad c_k^\dagger=N^{-1/2}\sum_l e^{ikl}c_l^\dagger,\quad (-\pi\le k<\pi), \quad (6)$$

we have

$$Kc_k^\delta K^{-1}=c_{k^r}^{-\delta}, \quad (7a)$$

$$Rc_k^\delta R^{-1}=c_{-k^r}^{-\delta}, \quad (7b)$$

where

$$c_k^\delta\equiv c_k^\dagger,\quad \delta=1,\qquad \equiv c_k,\quad \delta=-1, \quad (8)$$

and

$$k^r\equiv k-\pi,\quad k\ge 0,\qquad \equiv k+\pi,\quad k<0. \quad (9)$$

Because of the translational symmetry and the fact that the z component of the total spin S^z commutes with H, the eigenstates are characterized by a wave vector and S^z. We now write an arbitrary eigenstate ψ with $S^z=m+S_0$ and the wave vector $k=q+k_0$ (mod 2π), where S_0 and k_0 characterize the ground-state ψ_0, as

$$\psi=A\psi_0, \quad (10)$$

A has the following general form:

$$A\equiv\sum_{n=0}^{\infty}\sum_{\{k\}}\sum_{\{\delta\}}a(1,2,\cdots,n)\Delta^0(\delta_1+\delta_2+\cdots+\delta_n-m)\times\Delta(\delta_1k_1+\delta_2k_2+\cdots+\delta_nk_n-q)c_{k_1}^{\delta_1}c_{k_2}^{\delta_2}\cdots c_{k_n}^{\delta_n}, \quad (11)$$

where the number j in the argument of a stands for δ_j and k_j, and

$$\Delta(x)\equiv\sum_{p=0,\pm1,\cdots}\Delta^p(x),\quad \Delta^p(x)\equiv1,\quad x=2\pi p,\qquad \equiv0,\quad \text{otherwise}, \quad (12)$$

and we have used the fact that each Fermi particle carries a unit spin. We also understand that all the wave

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[1] J. des Cloizeaux and J. J. Pearson, Phys. Rev. **128**, 2131 (1962).

[2] P. W. Anderson, Phys. Rev. **86**, 694 (1952); R. Kubo, *ibid.* **87**, 568 (1952).

[3] E. Lieb, T. Schultz, and D. Mattis, Ann. Phys. (N. Y.) **16**, 407 (1961).

[4] K. Kawasaki (to be published).

vectors are reduced to be within the first Brillouin zone $(-\pi, \pi)$.

Let U be K or R. Then, the eigenvalue equation (the ground-state energy is taken to be zero)

$$HA\psi_0 = \epsilon(m,q)A\psi_0\,, \tag{13}$$

is transformed by U into

$$H\hat{A}\hat{\psi}_0 = \epsilon(m,q)\hat{A}\hat{\psi}_0\,, \tag{14}$$

where

$$\hat{A} \equiv UAU^{-1}, \quad \hat{\psi}_0 \equiv U\psi_0\,. \tag{15}$$

Thus the properties of the new eigenstate $\hat{\psi} \equiv \hat{A}\hat{\psi}_0$ are contained in $\hat{A}$.[5]

Let us first consider the case when m is an odd number. Then n is also odd. By applying the transformation (7a) to (11), we easily see that the state $\hat{\psi}$ is characterized by $-m$ and $-q^r$. Thus by (14) we obtain

$$\epsilon(-m, -q^r) = \epsilon(m,q)\,. \tag{16}$$

Similarly the transformation (7b) yields

$$\epsilon(-m, q^r) = \epsilon(m,q)\,. \tag{17}$$

Equations (16) and (17) are the main results of the present note. If $\epsilon(m,q)$ is an even function of m as for the des Cloizeaux and Pearson spin waves, we conclude from (16), (17), and (9) that $\epsilon(m,q)$ is an even function of q and has a periodicity of π for odd m. For even m the similar reasoning leads to the relations of the form of (16) and (17) where q^r is replaced by q.

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[5] Here we assume that the excitation energy $\epsilon(m,q)$ is determined only by m and q and does not depend on the choice of the ground state. This the case if we have a nondegenerate ground state.

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Positron Annihilation in Diatomic Crystals*

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The angular correlation between the two photons created by annihilating positron-electron pairs in lattices with a basis is derived in various approximations. The effects of temperature as introduced through the momentum distribution of the positrons and through lattice vibrations are examined. Self-consistent electron wave functions with exchange are calculated for the LiH crystal in the cell approximation. The resulting x-ray structure factors are in close agreement with the recent extensive experimental data of Calder *et al.* The positron wave function is obtained in the same approximation and the momentum distribution of annihilating positron-electron pairs is calculated. The apparent discrepancy noted by Stewart and March between their angular-correlation data and the electron density distribution in the LiH crystal consistent with the x-ray structure factors can be traced to the phase relations between the wave functions within the unit cell of a lattice with a basis.

INTRODUCTION

FREE thermalized positrons in a crystal annihilate almost exclusively via para-decay with electrons of opposite spin into two photons. Because of momentum conservation, the two photons are emitted in directions 180° apart in the center-of-mass system of the annihilating particles. If the center of mass is in motion relative to the laboratory, an observer sees angles between the photons which deviate from 180°. Therefore two-photon angular-correlation measurements give information on the momentum distribution of the annihilating positron-electron pairs, as was discussed in detail first by De Benedetti *et al.*[1] in 1950. Since then, angular correlation studies have been made by many investigators on a large number of substances.[2]

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[1] S. De Benedetti, C. E. Cowan, W. R. Konnecker, and H. Primakoff, Phys. Rev. **77**, 205 (1950).

[2] For recent reviews and extensive references, see P. R. Wallace, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1960), Vol. 10, p. 1; M. Deutsch and S. Berko, in *Alpha-, Beta- and Gamma-Ray Spectroscopy*, edited by K. Siegbahn (North-Holland Publishing Company, Amsterdam, 1965), Vol. 2, p. 1583.