COMPLEXES OF SEVERAL SPINS IN A LINEAR HEISENBERG CHAIN

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It is known that a canonical transformation reduces the Heisenberg spin Hamiltonian for a linear chain to the Hamiltonian for a lattice-like one-dimensional spinless Fermi gas with nearest-neighbor interaction only [1]. The sought Hamiltonian has the form

$$H = \frac{1}{2}\sum_{n=1}^{\infty} (a_n^+ a_{n+1} + a_{n+1}^+ a_n) + \gamma \sum_{n=1}^{N} a_n^+ a_n a_{n+1}^+ a_{n+1}, \qquad (1)$$

where the cyclic nature of the chain leads to the relation $a_{N+1} = a_1$ for the Fermi operators a_n, and γ characterizes the anisotropy of the initial spin Hamiltonian. The particle-number conservation law corresponds to conservation of the projection z of the total spin of the system. Assume that the number of spins L is finite (with $N \to \infty$). Following Bethe [2], we determine the self-energy and the eigenfunctions. The wave function of L particles is

$$\Psi_L = \sum_{n_1, n_2 ...=1}^{N} \Phi_L(n_1 n_2 \ldots n_L)\, a_{n_1}^+ a_{n_2}^+ \ldots a_{n_L}^+ |0\rangle, \qquad (2)$$

$$\Phi_L(n_1 n_2 \ldots n_L) = \sum_{P=1}^{L!} \exp i \left(\sum_{j=1}^{L} k_{p_j} n_j + \sum_{j<l} \phi_{p_j p_l} \right), \qquad n_1 < n_2 < \ldots < n_L. \qquad (3)$$

The summation is over all permutations of the "wave vectors" k_i ($i = 1, \ldots, L$), and p_j indicates the number produced at the location j as a result of the permutation P. The phases φ_{ij} satisfy the equations

$$N k_j = 2\pi\lambda_j + 2\sum_{l(\neq j)} \phi_{jl}, \qquad (4a)$$

$$\gamma \cos\left(\phi_{ij} + \frac{k_j - k_i}{2}\right) = \cos\phi_{ij} \cos\frac{k_i + k_j}{2}. \qquad (4b)$$

The λ_j are integers between 0 and N - 1, and φ_{ij} can be defined such that $-\pi/2 < \mathrm{Re}\,\varphi_{ij} < \pi/2$. Finally, the self-energy is given by

$$E = \sum_{i=1}^{L} \cos k_i. \qquad (5)$$

Equations (4) were solved for a system of spins with finite density in a number of papers [2-4] under the assumption that the ground state corresponds to real k_i. This assumption, however, has not been regorously justified, and therefore the authors of the cited papers point to a possible significance of complex k_i. We shall investigate complex k_i by starting from a system having a finite number of coupled spins.

To solve (4) for a finite spin system we assume that the only large phases are φ_{12}, φ_{23}, φ_{34}, ..., $\varphi_{L-1,L}$. This assumption will be rigorously justified subsequently. We shall assume further without loss of generality that Im $\varphi_{r-1} > 0$. From the cyclic conditions (4a) it follows that

$$
\begin{aligned}
&2\,\mathrm{Im}\,\phi_{12} = N\,\mathrm{Im}\,k_1 = N\kappa_1,\\
&2\,\mathrm{Im}(\phi_{23}-\phi_{12}) = N\,\mathrm{Im}\,k_2 = N\kappa_2,\\
&\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\\
&-2\,\mathrm{Im}\,\phi_{L-1,L} = N\,\mathrm{Im}\,k_L = N\kappa_L,\\
&\kappa_1+\kappa_2+\ldots+\kappa_L = 0.
\end{aligned} \tag{6}
$$

Substituting the large phases in (4b) we get with an accuracy exponential in N

$$
\gamma e^{\frac{i k_i - k_i + 1}{2}} = \cos\frac{k_i + k_i + 1}{2} \qquad i = 1, 2, \ldots, L-1. \tag{7}
$$

It is necessary to add to these L - 1 equations the equation

$$
\sum_{i=1}^{L} k_i = u = \frac{2\pi}{N}\sum_{i=1}^{N}\lambda_i, \tag{8}
$$

which follows from (4a). u is the total "momentum" of the spin system, and the self-energy enters in it as a parameter. The wave function $\Psi_L(n_1 n_2 \ldots n_L)$ is multiplied by exp(iuk) following the shift $n_i \to n_i + k$. The wave function should thus be characterized by a "momentum" u.

The solution of (7) should be given separately for three regions of γ, namely $\gamma > 1$, $\gamma < -1$, and $|\gamma| < 1$. We present the solution for the first case only: *)

$$
\gamma = \mathrm{ch}\, v > 1,
$$

$$
e^{ik_n} = \frac{\mathrm{sh}(L-n)v + e^{iu}\,\mathrm{sh}\, nv}{\mathrm{sh}(L-n+1)v + e^{iu}\,\mathrm{sh}(n-1)v}, \tag{9}
$$

$$
E_L^1(u) = L\,\mathrm{ch}\, v + \frac{\mathrm{sh}\, v}{\mathrm{sh}\, Lv}\cos u - \mathrm{sh}\, v\,\mathrm{cth}\, L v.
$$

In the case $|\gamma| < 1$, limitations are imposed on γ and u, but for lack of space we shall not write them out here.

*) sh ≡ sinh, ch ≡ cosh.

Substituting the obtained values of k_i in (4a), we can easily see that the remaining φ_{ij} are small compared with $\varphi_{k-1,k}$; this justifies the assumption made above.

We present without proof some consequences of (9):

1. When $\gamma < -1$, the bound states of L particles have an energy lower than that of L - 1 bound particles plus one free particle (of course, for the same value of u).

2. When $\gamma > 1$, the bound states of L particles have an energy higher than that of L - 1 bound particles plus one free particle.

3. When $|\gamma| < 1$, the bound states of L particles fall in the continuous spectrum (with exception of L = 2).

4. Summation over the permutations yields for the wave function of the bound state (3) only one term, $\exp i(k_1 n_1 + \ldots + k_L n_L)$.

5. When $|\gamma| > 1$ the complex is rigid, i.e., the probability of a hole appearing in the middle of the complex is negligible. Holes have a noticeable probability of occurrence only at the ends of the complex.

6. When $|\gamma| \leq 1$ the complex becomes brittle, i.e., states with a hole inside the complex are possible.

7. As $L \to \infty$, we get $E = L\gamma$ for all γ and the particle density in the complex tends to unity.

[1] S. Rodriguez, Phys. Rev. 116, 1474 (1959).

[2] H. Bethe, Z. Physik 71, 205 (1931).

[3] R. Orbach, Phys. Rev. 112, 309 (1958).

[4] R. Griffiths, ibid. 133A, 768 (1964).

[5] I. des Cloizeaux and I. Pearson, ibid. 128, 2131 (1962).

ANOMALOUS DIFFUSE SMALL-ANGLE MOSSBAUER SCATTERING IN CRYSTALS

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Bragg scattering of x rays in crystals is known to be accompanied by anomalous diffuse scattering in a narrow angle interval near the diffraction maximum (which corresponds to a wave-vector direction $\underset{\sim}{k}_1 = \underset{\sim}{k} + \underset{\sim}{K}$, where $\underset{\sim}{K}$ is the reciprocal-lattice vector). The differential scattering cross section is proportional here to $1/\kappa^2$, where $\kappa = \underset{\sim}{k}' - \underset{\sim}{k}_1$ (cf., e.g., [1]). Physically this is due to the periodicity of the phonon spectrum in the reciprocal-lattice space, whereby particle scattering in a regular crystal can always excite phonons of extremely low frequencies and yet effect an appreciable momentum transfer.

One the other hand, although low-frequency phonons are excited in small-angle scattering, there is no anomalous scattering, since the scattering cross section is proportional to the square of the momentum transfer. This result seems perfectly general at first glance.