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On spectral properties of the uniaxially anisotropic Heisenberg Hamiltonian

I. V. Krasovsky

Department of Physics, Kharkov State University, 4 Svoboda Square, Kharkov 310077, Ukraine

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The uniaxially anisotropic Heisenberg Hamiltonian H is considered, which describes a simple lattice of spins and incorporates first-nearest, ..., m-nearest neighbour interactions under the condition that $J_j \alpha_j \geq 0$, $j = 1, ..., m$, where J_j, α_j are the exchange and anisotropy constants of the j-th shell of neighbours, respectively. It is proved that, there are no bound states in the two-magnon space above the band of the continuous spectrum of H and, for the XY model, there are no two-magnon bound states at all.

Consider the following Hamiltonian of a simple periodic lattice of spins s:

$$H = \sum_{j=1}^{m} J_j h(j) ,$$

$$h(j) = -\frac{1}{2s} \sum_{\mathrm{i}, \vec{\delta}_j} [S_{\mathrm{i}}^{+} S_{\mathrm{i}+\vec{\delta}_j}^{-} + \alpha_j (S_{\mathrm{i}}^{z} S_{\mathrm{i}+\vec{\delta}_j}^{z} - s^2)] .$$

$$J_j \alpha_j \geq 0 , \; j = 1, ..., m ,$$

where the summation extends over all N lattice vectors **i** and over the vectors $\vec{\delta}_j$ connecting an atom with its j-nearest neighbours. For convenience, an additive constant is chosen so that $H|0\rangle = 0$, where $|0\rangle$ is the state of total spin alignment ($S_{\mathrm{i}}^{z}|0\rangle = s|0\rangle \, \forall \, \mathrm{i}$), and the Hamiltonian is divided by s.

The two-magnon space Γ_2, which is invariant under H is made up of the vectors $D(\mathrm{i}, \mathrm{j}) = S_{\mathrm{i}}^{-} S_{\mathrm{j}}^{-}|0\rangle / F$, where the norm factor $F = 2s$ if $\mathrm{i} \neq \mathrm{j}$, and $2\sqrt{s(2s-1)}$ otherwise.

The subspace of Γ_2 corresponding to the momentum **k** (we denote it by $\Gamma_{2\mathbf{k}}$) is spanned by the vectors

$$\varphi(\mathbf{q}) = (1/\sqrt{N}) \sum_{\mathbf{m}} e^{i\mathbf{k}\mathbf{m}} D(\mathbf{m}, \mathbf{m}+\mathbf{q}) e^{i\mathbf{k}\mathbf{q}/2} ,$$

where the summation is carried out over all lattice vectors **m**.

The analytical solutions of the spectral problem for H in $\Gamma_{2\mathbf{k}}$ are available only in a few simple cases (see, e.g., Ref. 1,2). In this connection, it appears interesting to investigate the general properties of the spectrum of H. The purpose of the present work is to solve part of this problem by comparing the spectrum of H with the well-known spectrum of the Hamiltonian $\Im$ *describing noninteracting magnons.*

We introduce $\Im$ as usual (e.g., Ref. 3): Consider the space $\mathrm{Sym}\,\Gamma_1^2$, i.e. the symmetric tensor product of two one-magnon spaces Γ_1, spanned by

$$\psi(\mathrm{i}, \mathrm{j}) = (S_{\mathrm{i}}^{-}|0\rangle \otimes S_{\mathrm{j}}^{-}|0\rangle + S_{\mathrm{j}}^{-}|0\rangle \otimes S_{\mathrm{i}}^{-}|0\rangle)/2sM ,$$

were $M = 2$ if $\mathrm{i} = \mathrm{j}$ and $\sqrt{2}$ otherwise. Then $\Im$ in $\mathrm{Sym}\,\Gamma_1^2$: $\Im = H_1 \otimes I + I \otimes H_1$, where H_1 is H acting in Γ_1, and I is the unity operator. Let us classify the eigenvalues of $\Im$ by the total momentum **k**. Then, accordingly,

$$\Im = \sum_{\mathbf{k}} \oplus \Im_{\mathbf{k}} ,$$

where $\Im_{\mathbf{k}}$ has the eigenvalues (which condense into an interval of the continuous spectrum* as $N \to \infty$) $\varepsilon(\mathbf{k}_1) + \varepsilon(\mathbf{k}_2)$, $\mathbf{k} = \mathbf{k}_1 + \mathbf{k}_2$, and $\varepsilon(\mathbf{k})$ are solutions of the one-magnon problem. $\Im_{\mathbf{k}}$ acts in the subspace $(\mathrm{Sym}\,\Gamma_1^2)_{\mathbf{k}}$ spanned by the vectors

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* Continuous spectrum here is the set of nonisolated points of growth of the resolution of the identity and eigenvalues of infinite multiplicity.

$$\varphi'(\mathrm{q}) = (1/\sqrt{N}) \sum_{\mathrm{m}} \mathrm{e}^{i\mathrm{km}} \psi(\mathrm{m}, \mathrm{m}+\mathrm{q}) \mathrm{e}^{i\mathrm{kq}/2} .$$

We note that $\Gamma_{2\mathbf{k}}$ is isomorphic with $P(s)(\mathrm{Sym}\,\Gamma_1^2)_{\mathbf{k}}$, where $P(s) = I$ if $s > 1/2$, and $P(1/2)$ is the orthogonal projection on the subspace spanned by vectors $\varphi'(\mathrm{q})$ with $\mathrm{q} \neq 0$. The choice of an isomorphism is apparent: $\varphi(\mathrm{q})$ corresponds to $P(s)\varphi'(\mathrm{q})$.

The main result here is the following theorem, which holds in the limit as $N \to \infty$.

Theorem. The spectrum of H in each $\Gamma_{2\mathbf{k}}$ includes a single interval of the continuous spectrum $C(H)$* and is bounded above by the least upper bound of $C(H)$; for $\alpha_j = 0$, $j = 1, \ldots, m$, i.e. the XY model, the spectrum is also bounded below by the greatest lower bound of $C(H)$. That is, there are no points of the discrete spectrum above $C(H)$, and, for the XY model, there is no discrete spectrum.

Proof. Operating with H on basis vectors $\varphi(\mathrm{q})$ and considering the limit as $N \to \infty$, we obtain the following representation for H in $\Gamma_{2\mathbf{k}}$:

$$H = L_{\mathbf{k}} + \beta V_1 + V_2 , \tag{1}$$

were $L_{\mathbf{k}}$ coincides with $P(s)\Im_{\mathbf{k}} P(s)$ in the above established isomorphism between $\Gamma_{2\mathbf{k}}$ and $P(s)(\mathrm{Sym}\,\Gamma_1^2)_{\mathbf{k}}$;

$$V_1\varphi(0) = \sum_{j=1}^{m} J_j \sum_{\vec{\delta}_j'} 2\cos(\mathrm{k}\vec{\delta}_j'/2)\varphi(\vec{\delta}_j') ,$$

$$V_1\varphi(\vec{\delta}_j') = J_j 2\cos(\mathrm{k}\vec{\delta}_j'/2)\varphi(0) ,$$

$$V_1\varphi(\mathrm{q}) = 0 \quad \text{if} \quad \mathrm{q} \neq 0, \vec{\delta}_j' ;$$

$$\beta = \sqrt{2} - \sqrt{2(1 - 1/2s)} \quad (V_1 = 0 \text{ if } s = 1/2) ;$$

$$V_2\varphi(\vec{\delta}_j') = -(J_j\alpha_j/s)\varphi(\vec{\delta}_j') ,$$

$$V_2\varphi(\mathrm{q}) = 0 \quad \text{if} \quad \mathrm{q} \neq \vec{\delta}_j' ,$$

where the prime indicates that $\vec{\delta}_j'$ take values in a halfspace [since $\varphi(\mathrm{q}) = \varphi(-\mathrm{q})$].

Since H coincides with the self-adjoint $\Im_{\mathbf{k}}$ in the isomorphism up to a finite-dimensional perturbation, we see by the Weyl theorem that $C(H)$ coincides with the spectrum of $\Im_{\mathbf{k}}$. Thus, taking it into account that, as is easy to show, the spectra of $n \times n$ truncated matrices $H_n(\Im_{\mathbf{k}n})$ represented in the basis of vectors $\varphi(\mathrm{q})$ [$\varphi'(\mathrm{q})$] converge to the spectrum of $H(\Im_{\mathbf{k}})$ as $n \to \infty$, it remains for us to prove the following statement for n greater than the dimensionality of $\beta V_1 + V_2$: The spectrum of H_n is bounded above by the maximum eigenvalue of $\Im_{\mathbf{k}n}$; for $\alpha_j = 0$, $j = 1, \ldots, m$, it is also bounded below by the minimum eigenvalue of $\Im_{\mathbf{k}n}$.

For $s = 1/2$, this statement is proved straightforwardly by the variational principle since $V_1 = 0$ and V_2 has only nonpositive eigenvalues.

In order to prove the theorem for $s > 1/2$, we note first of all that $X(\sqrt{2}) = L_{\mathbf{k}n} + \sqrt{2}V_1$ is represented in the basis of vectors $\varphi(\mathrm{q})$ as the direct sum of matrices of two operators, one of which coincides with $\Im_{\mathbf{k}n}$ restricted to the subspace spanned by $\varphi'(0)$, the other, with $\Im_{\mathbf{k}n}$ restricted to the orthogonal complement of the first subspace to the whole space where $\Im_{\mathbf{k}n}$ acts. Hence, the spectrum of $X(\sqrt{2})$ lies between the minimum and the maximum eigenvalues of $\Im_{\mathbf{k}n}$. Now considering the representation

$$X(\beta) = L_{\mathbf{k}n} + \beta V_1 = L_{\mathbf{k}n} + \gamma\sqrt{2}V_1 =$$

$$= \gamma X(\sqrt{2}) + (1 - \gamma)L_{\mathbf{k}n} , \tag{2}$$

$$\gamma = \beta/\sqrt{2} = 1 - \sqrt{1 - 1/2s}$$

and again using the variational principle, we see, since $0 \leq \gamma \leq 1$, that the spectrum of $X(\beta)$ lies between the minimum and the maximum eigenvalues of $\Im_{\mathbf{k}n}$. The complete proof follows from the fact that $H_n = X(\beta) + V_2$ and eigenvalues of V_2 are nonpositive.

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* We derive this known fact below for consistency.