Approximating parabolas as natural bounds of Heisenberg spectra: Reply on the comment of O. Waldmann

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PACS. 75.10.Jm – Quantized spin models.

O. Waldmann [1] has shown that some spin systems, which fulfill the condition of a weakly homogeneous coupling matrix, have a spectrum whose minimal energies $E_{\min}(S)$, or maximal energies $E_{\max}(S)$, are rather poorly approximated by a quadratic dependence on the total spin quantum number. We comment on this observation and provide the new argument that, under certain conditions, the approximating parabolas appear as natural bounds of the spectrum generated by spin coherent states.

In our article [2] we demonstrated that the spectrum of interacting spin systems, with Hamiltonians of the following form $\underset{\sim}{H} \equiv \sum_{\mu\nu} J_{\mu\nu} \underset{\sim}{\vec{s}}_\mu \cdot \underset{\sim}{\vec{s}}_\nu$, is bounded by an upper and a lower parabola, i.e. all energy eigenvalues lie between two curves which depend quadratically on the total spin quantum number S. This proof is rigorous and general and assumes only that the coupling constants $J_{\mu\nu}$ satisfy $J_{\mu\nu} = J_{\nu\mu}, J_{\mu\mu} = 0, j \equiv \sum_\nu J_{\mu\nu}$, with j being independent of μ. The latter is a kind of weak homogeneity assumption. In our notation $\underset{\sim}{\vec{s}}_\mu$ are single-spin operators of length s.

In the last section of our article [2] we also reported that the bounding parabolas when shifted by an appropriate amount can provide reasonable approximations ("approximating parabolas") to the boundaries of the exact energy spectrum for certain Heisenberg spin systems. Whereas the bounding parabolas follow rigorously from the assumptions, we made no such claim for the displaced "approximating parabolas". In fact, Waldmann [1] has provided several interesting examples of Heisenberg spin systems where the exact minimal energies $E_{\min}(S)$, or maximal energies $E_{\max}(S)$, are not accurately approximated by a quadratic dependence on the total spin quantum number S, even though the bounding parabolas do apply for those systems since the requirements are met. The observations of [1] are valuable in the sense that they help to clarify the conditions under which rotational bands, which are rather frequently observed [3–5], appear in magnetic systems.

In order to show that the approximating parabolas appear as natural bounds of the spectrum generated by spin coherent states, we first consider the convex set

$$E_{\text{qm}} \equiv \left\{ \left(\mathrm{Tr}\left\{ \underset{\sim}{H} \underset{\sim}{W} \right\}, \mathrm{Tr}\left\{ \underset{\sim}{\vec{S}}^2 \underset{\sim}{W} \right\} \right) \middle| \underset{\sim}{W} \text{ statistical operator} \right\} \subset \mathbb{R}^2 \ , \tag{1}$$

and its subset

$$E_{\text{cl}} = \left\{ \left(\langle\, \Omega \,|\, \underset{\sim}{H} \,|\, \Omega \,\rangle, \langle\, \Omega \,|\, \underset{\sim}{\vec{S}}^2 \,|\, \Omega \,\rangle, \right) \middle| \,|\, \Omega \,\rangle \text{ spin coherent product state} \right\} \subset \mathbb{R}^2 \ . \tag{2}$$

Here $|\,\Omega\,\rangle$ denotes any tensor product of N spin coherent states $|\,\vec{\Omega}_i\,\rangle, i = 1, \dots, N$. The $\vec{\Omega}_i$ are vectors parameterizing each spin coherent state by a unit vector pointing along the expected direction of the spin, i.e. $\langle\,\vec{\Omega}_i\,|\,\underset{\sim}{\vec{s}}\,|\,\vec{\Omega}_i\,\rangle = s\,\vec{\Omega}_i$. Note that for Heisenberg Hamiltonians $\langle\,\Omega\,|\,\underset{\sim}{H}\,|\,\Omega\,\rangle = s^2 h(\Omega)$, where $h(\Omega)$ denotes the classical Hamiltonian [6], whereas $\langle\,\Omega\,|\,\underset{\sim}{\vec{S}}^2\,|\,\Omega\,\rangle = S_{\text{cl}}^2 + N\,s$, $\quad S_{\text{cl}}^2 = s^2\left(\sum_i \vec{\Omega}_i\right)^2$. Denote by $\tilde{E}_{\min}(S)$ the minimum of all E for which $(E, S(S+1)) \in E_{\text{qm}}$. It is clear that $\tilde{E}_{\min}(S) \le E_{\min}(S)$, where $E_{\min}(S)$ denotes the minimal eigenvalue of $\underset{\sim}{H}$ within the subspace of total spin quantum number S. Analogously, $\tilde{E}_{\max}(S) \ge E_{\max}(S)$.

Using similar arguments as Berezin and Lieb [7,8] one can prove the following theorem [9].

Theorem 1 *Let the Hamilton operator be of the given form given and assume that* $E^{cl}_{min}(S_{cl}) \ge \frac{j - j_{min}}{N} S_{cl}^2 + j_{min} N s^2$, *with* j_{min} *being the minimal eigenvalue of the matrix* $(J_{\mu\nu})$. *Then for* $S(S+1) \ge N\,s$ *there holds* $\tilde{E}_{min}(S) \le p_L(S) \equiv \frac{j - j_{min}}{N} S(S+1) + j_{min}(N\,s^2 + s) - j\,s$, *where* $p_L(S)$ *coincides with the lower approximating parabola of Ref.* [2].

An analogous result can be proven which yields a lower bound for $\tilde{E}_{\max}(S)$. The assumption made above is fulfilled for a large class of spin systems, especially for weakly homogeneous systems, including the examples given in Refs. [2,5]. This theorem, to some extent, explains the good approximation of the true boundaries of the spectrum by the shifted parabolas for those systems where $\tilde{E}_{\min}(S)$ and $E_{\min}(S)$ are close (analogously for the maxima). Theorem 1 would yield exact bounds for the spectrum if the polygon P with the vertices $(E_{\min}(S), S(S+1))$ and $(E_{\max}(S), S(S+1))$ would circumscribe a convex figure, which then would be identical with E_{qm}. Actually the polygon P seems to be slightly concave for the examples we considered.

The interesting case (a) of [1] shows a lowest level in the $(S = 0)$-sector of the spectrum which is above the approximating parabola and thus might appear to contradict our findings. However, there is no contradiction since for such small total spin quantum numbers the condition $S(S+1) \ge N\,s$ cannot be fulfilled and thus the true minimal energy may lie above the approximating parabola.

Summarizing, our approximating parabolas appear as natural bounds of the convex hull of the spectrum generated by spin coherent states under the conditions specified by Theorem 1. Therefore, these parabolas are of genuine classical origin, as correctly pointed out by O. Waldmann. But this does not mean that they are necessarily poor approximations. It only shows that in those cases where the approximations by parabolas are reasonable the shape of the quantal spectrum is essentially determined by classical physics.

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